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Proteus Two-Dimensional Navier-Stokes Computer Code—Version 2.0

Volume 3—Programmer's Reference

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PROTEUS TWO-DIMENSIONAL NAVIER-STOKES COMPUTER CODE - VERSION 2.0

Volume 3 - Programmer's Reference

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SUMMARY

A computer code called *Proteus* has been developed to solve the two-dimensional planar or axisymmetric, Reynolds-averaged, unsteady compressible Navier-Stokes equations in strong conservation law form. The objective in this effort has been to develop a code for aerospace propulsion applications that is easy to use and easy to modify. Code readability, modularity, and documentation have been emphasized.

The governing equations are written in Cartesian coordinates and transformed into generalized nonorthogonal body-fitted coordinates. They are solved by marching in time using a fully-coupled alternating-direction-implicit solution procedure with generalized first- or second-order time differencing. The boundary conditions are also treated implicitly, and may be steady or unsteady. Spatially periodic boundary conditions are also available. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. Turbulence is modeled using either an algebraic or two-equation eddy viscosity model.

The program contains many operating options. The governing equations may be solved for two-dimensional planar flow, or axisymmetric flow with or without swirl. The thin-layer or Euler equations may be solved as subsets of the Navier-Stokes equations. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used to damp pre- and post-shock oscillations in supersonic flow and to minimize odd-even decoupling caused by central spatial differencing of the convective terms in high Reynolds number flow. Several time step options are available for convergence acceleration, including a locally variable time step and global time step cycling. Simple Cartesian or polar grids may be generated internally by the program. More complex geometries require an externally generated computational coordinate system.

The documentation is divided into three volumes. Volume 1 is the Analysis Description, and presents the equations and solution procedure used in *Proteus*. It describes in detail the governing equations, the turbulence model, the linearization of the equations and boundary conditions, the time and space differencing formulas, the ADI solution procedure, and the artificial viscosity models. Volume 2 is the User's Guide, and contains information needed to run the program. It describes the program's general features, the input and output, the procedure for setting up initial conditions, the computer resource requirements, the diagnostic messages that may be generated, the job control language used to run the program, and several test cases. Volume 3, the current volume, is the Programmer's Reference, and contains detailed information useful when modifying the program. It describes the program structure, the Fortran variables stored in common blocks, and the details of each subprogram.

Version 1.0 of the two-dimensional *Proteus* code was released in late 1989. The current documentation covers Version 2.0, released in early 1992.

1.0 INTRODUCTION

Much of the effort in applied computational fluid dynamics consists of modifying an existing program for whatever geometries and flow regimes are of current interest to the researcher. Unfortunately, nearly all of the available non-proprietary programs were started as research projects with the emphasis on demonstrating the numerical algorithm rather than ease of use or ease of modification. The developers usually intend to clean up and formally document the program, but the immediate need to extend it to new geometries and flow regimes takes precedence.

The result is often a haphazard collection of poorly written code without any consistent structure. An extensively modified program may not even perform as expected under certain combinations of operating options. Each new user must invest considerable time and effort in attempting to understand the underlying structure of the program if intending to do anything more than run standard test cases with it. The user's subsequent modifications further obscure the program structure and therefore make it even more difficult for others to understand.

The *Proteus* two-dimensional Navier-Stokes computer program is a user-oriented and easily-modifiable flow analysis program for aerospace propulsion applications. Readability, modularity, and documentation were primary objectives during its development. The entire program was specified, designed, and implemented in a controlled, systematic manner. Strict programming standards were enforced by immediate peer review of code modules; Kernighan and Plauger (1978) provided many useful ideas about consistent programming style. Every subroutine contains an extensive comment section describing the purpose, input variables, output variables, and calling sequence of the subroutine. With just three clearly-defined exceptions, the entire program is written in ANSI standard Fortran 77 to enhance portability. A master version of the program is maintained and periodically updated with corrections, as well as extensions of general interest (e.g., turbulence models.)

The *Proteus* program solves the unsteady, compressible, Reynolds-averaged Navier-Stokes equations in strong conservation law form. The governing equations are written in Cartesian coordinates and transformed into generalized nonorthogonal body-fitted coordinates. They are solved by marching in time using a fully-coupled alternating-direction-implicit (ADI) scheme with generalized time and space differencing (Briley and McDonald, 1977; Beam and Warming, 1978). Turbulence is modeled using either the Baldwin and Lomax (1978) algebraic eddy-viscosity model or the Chien (1982) two-equation model. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. The boundary conditions are treated implicitly, and may be steady or unsteady. Spatially periodic boundary conditions are also available.

The program contains many operating options. The governing equations may be solved for two-dimensional planar flow, or axisymmetric flow with or without swirl. The thin-layer or Euler equations may be solved as subsets of the Navier-Stokes equations. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used to damp pre- and post-shock oscillations in supersonic flow and to minimize odd-even decoupling caused by central spatial differencing of the convective terms in high Reynolds number flow. Several time step options are available for convergence acceleration, including a locally variable time step and global time step cycling. Simple grids may be generated internally by the program; more complex geometries require external grid generation, such as that developed by Chen and Schwab (1988).

The documentation is divided into three volumes. Volume 1 is the Analysis Description, and presents the equations and solution procedure used in *Proteus*. It describes in detail the governing equations, the turbulence model, the linearization of the equations and boundary conditions, the time and space differencing formulas, the ADI solution procedure, and the artificial viscosity models. Volume 2 is the User's Guide, and contains information needed to run the program. It describes the program's general features, the input and output, the procedure for setting up initial conditions, the computer resource requirements,

the diagnostic messages that may be generated, the job control language used to run the program, and several test cases. Volume 3, the current volume, is the Programmer's Reference, and contains detailed information useful when modifying the program. It describes the program structure, the Fortran variables stored in common blocks, and the details of each subprogram.

Version 1.0 of the two-dimensional *Proteus* code was released in late 1989 (Towne, Schwab, Benson, and Suresh, 1990). The current documentation covers Version 2.0, released in early 1992.

The authors would like to acknowledge the significant contributions made by their co-workers. Tom Benson provided part of the original impetus for the development of *Proteus*, and did the original coding of the block tri-diagonal inversion routines. Simon Chen did the original coding of the Baldwin-Lomax turbulence model, and consulted in the implementation of the nonlinear coefficient artificial viscosity model. William Kunik developed the original code for computing the metrics of the generalized nonorthogonal grid transformation. Frank Molls has created separate diagonalized and patched-grid versions of the code. Ambady Suresh did the original coding for the second-order time differencing and for the nonlinear coefficient artificial viscosity model. These people, along with Dick Cavicchi, Julie Conley, Jason Solbeck, and Pat Zeman, have also run many debugging and verification cases.

2.0 PROGRAM STRUCTURE

2.1 FLOW CHART

In this section, a flow chart is presented showing the overall sequence of tasks performed by the two-dimensional *Proteus* computer code. Depending on the various options used in a particular run, of course, some of the elements in the chart may be skipped.

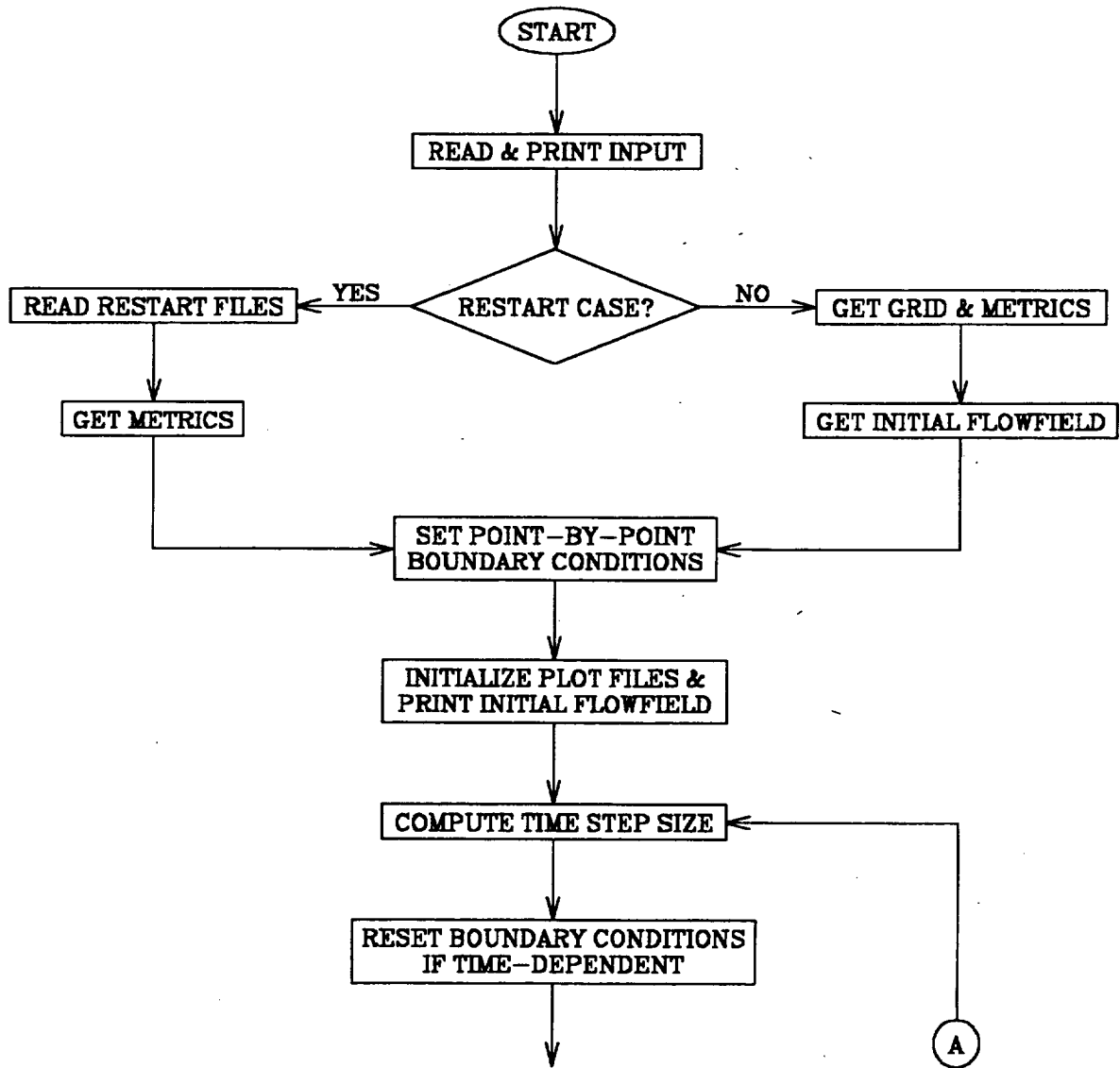


Figure 2.1 - Flow chart for the 2-D Proteus computer code.

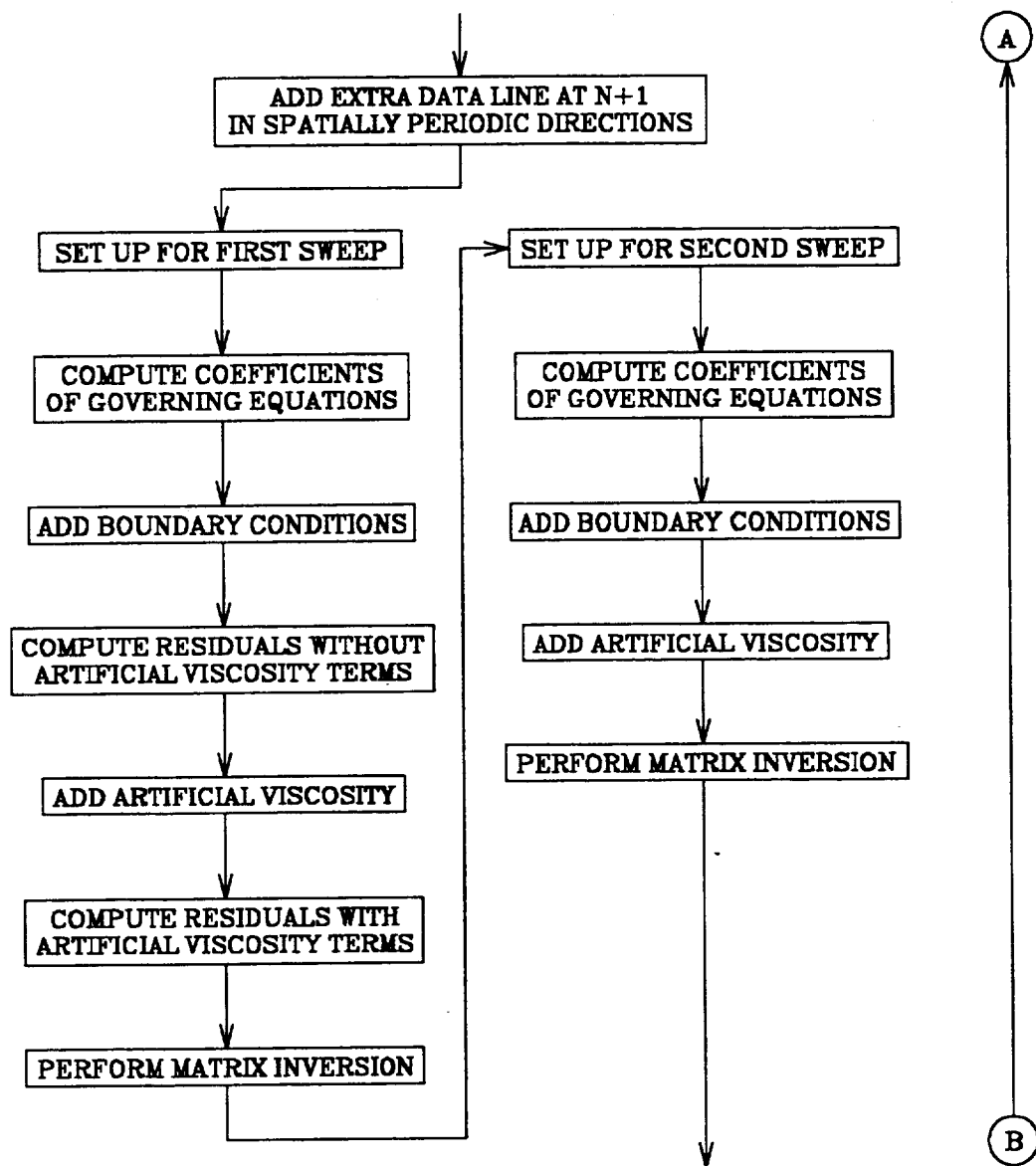


Figure 2.1 - Continued.

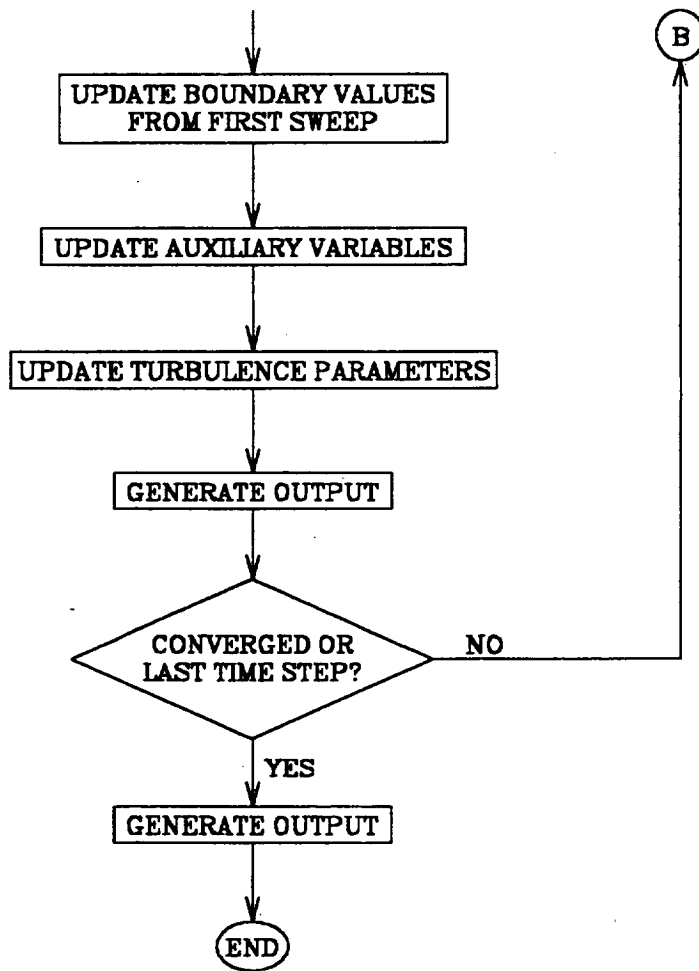


Figure 2.1 - Concluded.

2.2 SUBPROGRAM CALLING TREE

In this section, the calling sequence for the various subprograms in the *Proteus* 2-D code is shown using a tree structure. The subheadings correspond to the elements of the flow chart shown in the previous section. The main program, listed in the first column, calls the subprograms in the second column, which in turn call those in the third column, etc.¹ For any given case, of course, some of these routines will not be used. The subprograms needed for a particular case will depend on the combination of input parameters being used. The individual subprograms are described in detail in Section 4.0.

INITIALIZATION					
Read and print input.					
MAIN	INPUT	ISAMAX			
Get grid and metric parameters.					
MAIN	GEOM	PAK METS	ROBTS CUBIC OUTPUT	PRTOUT	
Get initial flow field.					
MAIN	INITC	REST INIT FTEMP EQSTAT TURBBL YPLUSN	METS VORTEX BLOUT1 BLIN1 BLOUT2 BLIN2 TURBBL YPLUSN PRODC VORTEX	ISAMAX ISAMIN ISRCHEQ ISRCHEQ ISAMAX ISAMIN ISRCHEQ ISRCHEQ VORTEX BLOUT1 BLIN1 BLOUT2 BLIN2 VORTEX	ISAMAX ISAMIN ISRCHEQ ISRCHEQ ISAMAX ISAMIN ISRCHEQ ISRCHEQ
Set point-by-point boundary condition values.					
MAIN	BCSET				

¹ Throughout this Programmer's Reference, elements of the Fortran language, such as input variables and subprogram names, are printed in the text using uppercase letters. However, in most implementations, Fortran is case-insensitive. The *Proteus* source code itself is written in lowercase.

[illegible]

Compute residuals without artificial viscosity terms (sweep 1 only.)					
MAIN	EXEC	RESID	SNRM2 ISAMAX SASUM		
Add artificial viscosity.					
MAIN	EXEC	AVISC1 AVISC2	BLKOUT BLKOUT		
Compute residuals with artificial viscosity terms (sweep 1 only.)					
MAIN	EXEC	RESID	SNRM2 ISAMAX SASUM		
SOLVE DIFFERENCE EQUATIONS					
Perform matrix inversion.					
MAIN	EXEC	ADI	BLKOUT BLK3P BLK3	FILTER	ISAMAX ISRCHEQ BLKOUT
			BLK4P BLK4	FILTER	ISAMAX ISRCHEQ BLKOUT
			BLK5P BLK5	FILTER	ISAMAX ISRCHEQ BLKOUT
		UPDATE			

Update boundary values from first sweep.					
MAIN	EXEC	BVUP	EQSTAT BCGEN	BCQ BCUVEL BCVVEL BCWVEL BCPRES BCTEMP BCDENS BCVDIR BCF ISRCHEQ BLKOUT	BCMET BCGRAD BCMET BCGRAD BCMET BCGRAD BCMET BCGRAD BCMET BCGRAD BCMET BCGRAD BCMET BCGRAD BCMET BCFLIN BCMET
			SGEFA SGESL		
FINISH TIME STEP AND CHECK RESULTS					
Update auxiliary variables.					
MAIN	EQSTAT FTEMP				
Update turbulence parameters.					
MAIN	TURBBL TURBCH	VORTEX BLOUT1 BLIN1 BLOUT2 BLIN2 YPLUSN PRODCT EXECT	ISAMAX ISAMIN ISRCHEQ ISRCHEQ ISAMAX ISAMIN ISRCHEQ ISRCHEQ VORTEX PERIOD COEFS1 BLK2P BLK2 COEFS2 BLK2P BLK2 UPDTKE		
Check for convergence, and get CPU time remaining.					
MAIN	CONV TREMAIN	ISAMAX			

GENERATE OUTPUT					
Print flow field output.					
MAIN	OUTPUT OUTW	VORTEX PRTOUT			
Write plot and restart files.					
MAIN	PLOT REST				
Print convergence history.					
MAIN	PRTHST				

2.3 PROGRAMMING CONVENTIONS AND NOTES

2.3.1 Computer & Language

At NASA Lewis Research Center, *Proteus* is normally run on a Cray X-MP or Y-MP computer. With just three known exceptions, it is written entirely in ANSI standard Fortran 77 as described in the *CF77 Compiling System, Volume 1: Fortran Reference Manual* (Cray Research, Inc., 1990). The first exception is the use of namelist input. With namelist input, it's relatively easy to create and/or modify input files, to read the resulting files, and to program default values. Since most Fortran compilers allow namelist input, its use is not considered a serious problem. The second exception is the use of *CALL statements to include *COMDECK's, which contain the labeled common blocks, in most of the subprograms. This is a Cray UPDATE feature, and therefore the source code must be processed by UPDATE to create a file that can be compiled.² UPDATE is described in the *UPDATE Reference Manual* (Cray Research, Inc., 1988). Since using the *CALL statements results in cleaner, more readable code, and since many computer systems have an analogous feature, the *CALL statements were left in the program. The third exception is the use of lowercase alphabetic characters in the Fortran source code. This makes the code easier to read, and is a common extension to Fortran 77.

Several library subroutines are called by *Proteus*. SGEFA and SGESL are Cray versions of LINPACK routines. SASUM and SNRM2 are Cray Basic Linear Algebra Subprograms (BLAS). ISAMAX, ISAMIN, and ISRCHEQ are Cray search routines. TREMAIN is a Cray Fortran library routine. All of these routines are described in detail in Section 4.0. In addition, SGEFA and SGESL are described in *Volume 3: UNICOS Math and Scientific Library Reference Manual* (Cray Research, Inc., 1989b) and by Dongarra, Moler, Bunch, and Stewart (1979); SASUM, SNRM2, ISAMAX, ISAMIN, and ISRCHEQ are described in *Volume 3: UNICOS Math and Scientific Library Reference Manual* (Cray Research, Inc., 1989b); and TREMAIN is described in *Volume 1: UNICOS Fortran Library Reference Manual* (Cray Research, Inc., 1989a).

The *Proteus* code is highly vectorized for optimal performance on the Cray. The coefficient generation is vectorized in the ADI sweep direction. Since the coefficient matrix is block tridiagonal, the equations are solved using the Thomas algorithm. This algorithm is recursive, and therefore cannot be vectorized in the sweep direction. However, by storing the coefficients and source terms in both coordinate directions, the algorithm can be vectorized in the non-sweep direction. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

² See the example in Section 8.1 of Volume 2.

2.3.2 Fortran Variables

Variable Names

In developing *Proteus*, code readability has been emphasized. We have therefore attempted to choose Fortran variable names that are meaningful. In general, they either match the notation used in the analysis description in Volume 1, or are in some way descriptive of the parameter being represented. For example, RHO, U, V, W, and ET are the Fortran variables representing the density ρ , the velocities u , v , and w , and the total energy per unit volume E_T .

Real and Integer Variables

In general, the type (real or integer) of the Fortran variables follows standard Fortran convention (i.e., those starting with I, J, K, L, M, or N are integer, and the remainder are real.) There are, however, several variables that would normally be integer but are explicitly declared to be real. These are noted in the input description in Section 3.0 of Volume 2, and in the description of common block variables in Section 3.0 of this volume.

Array Dimensions

Most Fortran arrays are dimensioned using dimensioning parameters. These parameters are set in COMDECK PARAMS1. This allows the code to be re-dimensioned simply by changing the appropriate parameters, and then recompiling the entire program. The dimensioning parameters are described in Section 6.2 of Volume 2.

Initialization

All of the input Fortran variables, plus some additional variables, are initialized in BLOCK DATA. Most of the input variables are initialized to their default values directly, but some are initialized to values that trigger the setting of default values in subroutine INPUT. On the Cray X-MP and Y-MP at NASA Lewis, all uninitialized variables have the value zero. There are no known instances in the *Proteus* code, however, in which a variable is used before it is assigned a value.

Nondimensionalization

In general, Fortran variables representing physical quantities, such as RHO, U, etc., are nondimensional. Two types of nondimensionalizing factors are used - *reference* conditions and *normalizing* conditions. The factors used to nondimensionalize the governing equations in Section 2.0 of Volume 1 are called *normalizing* conditions. These normalizing conditions are defined by six basic *reference* conditions, for length, velocity, temperature, density, viscosity, and thermal conductivity, which are specified by the user. The normalizing conditions used in *Proteus* are listed in Table 3-1 of Volume 2.

Note that for some variables, like pressure, the normalizing condition is dictated by the form of the governing equations once the six basic reference conditions are chosen. Unfortunately, some of these may not be physically meaningful or convenient for use in setting up input conditions. Therefore, some additional reference conditions are defined from the six user-supplied ones. The reference conditions are listed in Table 3-2 of Volume 2.

Throughout most of the *Proteus* code, physical variables are nondimensionalized by the normalizing conditions. For input and output, however, variables are nondimensionalized by the reference conditions because they are usually more physically meaningful for the user. The Fortran variables representing the reference conditions themselves are, of course, dimensional.

One-Dimensional Addressing of Two-Dimensional Arrays

In the solution algorithm used in *Proteus*, there are several instances in which the same steps must be followed in both ADI sweep directions. An example is the computation, in the COEFC, COEFX, COEFY, COEFZ, and COEFE routines, of the submatrices in the block tridiagonal coefficient matrix. These computations involve various flow variables, such as RHO, U, etc., and metric quantities, such as

XIX, XIY, etc. These are stored as two-dimensional arrays, with the two subscripts representing, in order, the indices in the computational ξ and η directions. For the first ADI sweep, values at various ξ indices are needed at a fixed η index. For the second ADI sweep, the reverse is true. In order to use the same coding for both sweeps, a scheme for one-dimensional addressing of a two-dimensional array has been used.³

In Fortran, multi-dimensional arrays are actually stored in memory as a one-dimensional sequence of values, with the first subscript incremented over its range first, then the second subscript, etc. We take advantage of this in *Proteus*. As a first step, the two-dimensional array is equivalenced to a one-dimensional array of the same total length. The one-dimensional array name is derived from the two-dimensional array name by adding a "1". Thus, letting F represent a typical two-dimensional array,

```
dimension f(n1p,n2p),f1(ntotp)
equivalence (f(1,1),f1(1))
```

where N1P and N2P are dimensioning parameters specifying the dimension size in the ξ and η directions, and NTOTP is a dimensioning parameter equal to N1P \times N2P. Next, we define a "step factor", which depends on the ADI sweep, and a "base index" which depends on the index in the non-sweep direction. For the first ADI sweep,

```
      istep = 1
      do 1000 i2 = 2,npt2-1
        iv = i2
        ibase = 1 + (i2-1)*n1p
        .
        .
        .
1000  continue
```

And for the second ADI sweep,

```
      istep = n1p
      do 2000 i1 = 2,npt1-1
        iv = i1
        ibase = i1
        .
        .
        .
2000  continue
```

In both of the above examples, the loop is in the non-sweep direction and IV therefore represents the index in the non-sweep direction. Nested inside this loop is a loop in the sweep direction. In this inner loop, we can compute the equivalent one-dimensional address for a location in a two-dimensional array from the step factor, the base index, and the index in the sweep direction. Thus, for either ADI sweep, the inner loop looks like

```
      do 100 i = 2,npts-1
        iim1 = ibase + istep*(i-2)
        ii   = ibase + istep*(i-1)
        iip1 = ibase + istep*i
        .
        .
        .
100  continue
```

where I represents the index in the sweep direction. With this coding, for the first sweep

³ An alternative would be to switch the order of the two subscripts in these arrays after each sweep. Since these arrays are used in many other areas of the code, this idea was discarded as being unnecessarily confusing. It should be noted, however, that there are some other arrays in *Proteus* in which the order of the two subscripts does switch between sweeps. This is described in the next subsection.

```

f1(iim1) = f(il-1,i2)
f1(ii ) = f(il ,i2)
f1(iip1) = f(il+1,i2)

```

And for the second sweep,

```

f1(iim1) = f(il,i2-1)
f1(ii ) = f(il,i2 )
f1(iip1) = f(il,i2+1)

```

Multi-Dimensional Addressing of One-Dimensional Arrays

As noted in the previous subsection, there are some arrays in *Proteus* in which the order of the first two subscripts does switch between ADI sweeps. These are the A, B, C, and S arrays, which represent the coefficient submatrices and the source term subvector, and the METX, METY, and METT arrays, which represent the metric coefficients in the sweep direction. (A, B, and C are actually four-dimensional arrays, with the third and fourth subscripts representing the equation and dependent variable, respectively. Similarly, S is actually a three-dimensional array, with the third subscript representing the equation. Only the first two subscripts switch between sweeps, however.) For these arrays, the first subscript is the index in the non-sweep direction (i.e., the η direction for the first sweep and the ξ direction for the second sweep), and the second is the index in the sweep direction (i.e., ξ for the first sweep and η for the second sweep.)

These multi-dimensional arrays are actually equivalenced to corresponding one-dimensional arrays, stored in common blocks NUM1 and METRIC1.⁴ The equivalence is done in subroutine EXEC, which manages the solution of the mean flow equations, and in subroutine EXECT, which manages the solution of the k - ϵ turbulence model equations. The multi-dimensional arrays and the appropriate dimensions, which depend on the ADI sweep, are then passed into lower level routines via the argument list. In the lower level routines they can then be referenced as normal, multi-dimensional arrays.

Thus, in subroutine EXEC, we have

```

dimension a(1,1,1,1),b(1,1,1,1),c(1,1,1,1),s(1,1,1)
equivalence (amat1(1),a(1,1,1,1)),(bmat1(1),b(1,1,1,1)),
$          (cmat1(1),c(1,1,1,1)),(svect1(1),s(1,1,1))
dimension metx(1,1),mety(1,1),mett(1,1)
equivalence (metx1(1),metx(1,1)),(mety1(1),mety(1,1)),
$          (mett1(1),mett(1,1))

```

Here METX1, METY1, and METT1 are one-dimensional arrays of length $N1P \times N2P$ stored in common block METRIC1. Similarly, AMAT1, BMAT1, CMAT1, and SVECT1 are one-dimensional arrays stored in common block NUM1. AMAT1, BMAT1, and CMAT1 are of length $N1P \times N2P \times NEQP \times NEQP$, and SVECT1 is of length $N1P \times N2P \times NEQP$.

Using COEFC as an example of a lower level routine, we have

```

subroutine coefc (a,b,c,s,metx,mety,mett,nvd,nptsd)
dimension a(nvd,nptsd,neqp,neqp),b(nvd,nptsd,neqp,neqp),
$          c(nvd,nptsd,neqp,neqp),s(nvd,nptsd,neqp)
dimension metx(nvd,nptsd),mety(nvd,nptsd),mett(nvd,nptsd)

```

where NVD and NPTSD are the dimensions in the non-sweep and sweep directions, respectively. For the first sweep, COEFC is thus called from EXEC as

```

call coefc (a,b,c,s,metx,mety,mett,n2p,n1p)

```

And for the second sweep, COEFC is called as

⁴ An alternative would be use the maximum of N1P and N2P as the size for both of the first two dimensions. In fact, this is what was done in earlier versions of *Proteus*. However, if N1P is significantly different from N2P, this is inefficient, requiring much more storage than the current procedure.

```
call coefc (a,b,c,s,metx,mety,mett,nlp,n2p)
```

Two-Level Storage

With the Beam-Warming time differencing scheme used in *Proteus*, the dependent variables RHO, U, V, W, and ET must be stored at two time levels. For convenience, T is also stored at two time levels. In the ADI solution procedure, RHO, U, etc. are at the known time level n . The corresponding variable at the other time level is denoted by adding an "L" to the variable name. Exactly which time level the "L" variable is at depends on the stage in the solution procedure. Letting F represent one of these variables, the time levels for F and FL are listed in the following table for the different stages of the solution procedure. Recall that * represents the intermediate time level after the first ADI sweep.

STAGE IN TIME STEP FROM LEVEL n TO $n + 1$	TIME LEVEL FOR F	TIME LEVEL FOR FL
From start to end of sweep 1	n	$n - 1$
From end of sweep 1 to end of sweep 2	n	*
From end of sweep 2 to update in EXEC	n	$n + 1$
From update in EXEC to start of next step	$n + 1$	n

DUMMY Array

For convenience, a two-dimensional array called DUMMY is stored in common block DUMMY1 and used as a temporary storage location in several areas of the code. This array is dimensioned N1P by N2P, the same as the flow variables, metrics, etc. DUMMY is used internally in subroutines CONV and RESID. It is also defined in subroutines BLIN2 and BLOUT2 for use in TURBBL, and in subroutine YPLUSN for use in subroutines COEFS1 and KEINIT. And finally, it is defined in subroutine OUTPUT and passed as an argument into subroutine PRTOUT. Details on its use are presented in the subroutine descriptions in Section 4.0.

3.0 COMMON BLOCKS

Transfer of data between routines in *Proteus* is primarily accomplished through the use of labeled common blocks. Each common block contains variables dealing with a particular aspect of the analysis, and is stored in a separate Cray COMDECK (Cray Research, Inc., 1988). The common block names are the same as the COMDECK names. These names also correspond to the names of the input namelists. All the variables in namelist BC are stored in common block BC1, etc. The Fortran variables in each common block are stored in alphabetical order.

3.1 COMMON BLOCK SUMMARY

<u>Block Name</u>	<u>Description</u>
BC1	Boundary condition parameters for the mean flow equations.
BC2	Boundary condition parameters for the k - ϵ equations.
DUMMY1	Scratch array.
FLOW1	Variables dealing with fluid properties and the flow being computed.
GMTRY1	Parameters defining the geometric configuration.
IC1	Variables needed for setting up initial conditions.
IO1	Parameters dealing with program input/output requirements.
METRIC1	Metrics of the nonorthogonal grid transformation, plus the Cartesian coordinates of the grid points.
NUM1	Parameters associated with the numerical method for the mean flow equations.
NUM2	Parameters associated with the numerical method for the k - ϵ equations.
RSTRT1	Parameters dealing with the restart option.
TIME1	Parameters dealing with the time step selection and convergence determination.
TITLE1	Descriptive title for case being run.
TURB1	Turbulence parameters.
TURB20	Parameters and constants associated with the k - ϵ equations.

3.2 COMMON VARIABLES LISTED ALPHABETICALLY

In this section all the *Proteus* Fortran variables stored in common blocks are defined, listed alphabetically by variable name. Those marked with an asterisk are input variables. More details on these variables may be found in Section 3.1 of Volume 2. The common block each variable is stored in is given in parentheses at the end of each definition. For subscripted variables, the subscripts are defined along with the variable, except for the subscripts I1 and I2, which are the indices i and j in the ξ and η directions, respectively, and run from 1 to N_1 and N_2 .

This list also includes the parameters used as array dimensions. These are not actually stored in a common block, but are stored in the Cray COMDECK PARAMS1. More details may be found in Section 6.2 of Volume 2.

Unless otherwise noted, all variables representing physical quantities are nondimensional. The nondimensionalizing procedure is described in Section 3.1.1 of Volume 2. The type (real or integer) of the variables follows standard Fortran convention, unless stated otherwise. (I.e., those starting with I, J, K, L, M, or N are integer, and the remainder are real.)

<u>Fortran Variable</u>	<u>Symbol</u>	<u>Definition</u>
A	A	See AMAT1. (NUM1)
AMAT1(I)	A	Subdiagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array A(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)
* APLUS	A^+	Van Driest damping constant in the inner and outer regions of the Baldwin-Lomax turbulence model. (TURB1)
B	B	See BMAT1. (NUM1)
BMAT1(I)	B	Diagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array B(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)
C	C	See CMAT1. (NUM1)
* CAVS2E(I)	$\varepsilon_E^{(2)}$ or κ_2	Second-order explicit artificial viscosity coefficient in constant coefficient model, or user-specified constant in nonlinear coefficient model. The subscript I = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* CAVS2I(I)	ε_I	Second-order implicit artificial viscosity coefficient in constant coefficient model. The subscript I = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* CAVS4E(I)	$\varepsilon_E^{(4)}$ or κ_4	Fourth-order explicit artificial viscosity coefficient in constant coefficient model, or user-specified constant in nonlinear coefficient model. The subscript I = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* CB	B	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbu-

		lence model, and in the inner region of the Spalding-Kleinstein turbulence model. (TURB1)
* CCLAU	K	Clauser constant used in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* CCP	C_{cp}	Constant used in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
CCP1-4	$C_{cp1} - C_{cp4}$	Constants in empirical formula for specific heat as a function of temperature. (FLOW1)
* CFL(I)		The ratio $\Delta\tau/\Delta\tau_{eff}$ where $\Delta\tau$ is the actual time step used in the implicit calculation and $\Delta\tau_{eff}$ is the allowable time step based on the Courant-Friedrichs-Lewy (CFL) criterion for explicit methods. I is the time step sequence number, and runs from 1 to NTSEQ. (TIME1)
* CFLMAX		Maximum allowed value of the CFL number. (TIME1)
* CFLMIN		Minimum allowed value of the CFL number. (TIME1)
CHGAVG(I)	ΔQ_{avg}	Maximum change in absolute value of the dependent variables, averaged over the last NITAVG time steps. ⁵ The subscript I = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (TIME1)
CHGMAX(I,J)	ΔQ_{max}	Maximum change in absolute value of the dependent variables over a single time step. ⁵ The subscript I = 1 to N_{eq} , corresponding to the N_{eq} dependent variables, and J = 1 to NITAVG, the number of time steps used in the moving average option for determining convergence. (TIME1)
* CHG1		Minimum change, in absolute value, that is allowed in any dependent variable before increasing the time step. ⁵ (TIME1)
* CHG2		Maximum change, in absolute value, that is allowed in any dependent variable before decreasing the time step. ⁵ (TIME1)
* CKLEB	C_{Kleb}	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* CKMIN	$(C_{Kleb})_{min}$	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
CK1-2	$C_{k1} - C_{k2}$	Constants in empirical formula for thermal conductivity coefficient as a function of temperature. (FLOW1)
CMAT1(I)	C	Superdiagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array C(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N. IV is the grid index in the "vectorized"

⁵ For the energy equation, the change in E_T is divided by $E_T = \rho_r \bar{R} T_r / (\gamma_r - 1) + u_r^2/2$, so that it is the same order of magnitude as the other conservation variables.

direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript $J = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations, and $K = 1$ to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)

* CMUR	C_{μ_r}	Constant used to compute C_μ in the turbulent viscosity formula for the k - ε equations. (TURB20)
CMU1-2	$C_{\mu 1} - C_{\mu 2}$	Constants in empirical formula for laminar viscosity coefficient as a function of temperature. (FLOW1)
* CNA	n	Exponent in the formula used to average the two outer region μ_t profiles that result when both boundaries in a coordinate direction are solid surfaces. (TURB1)
* CNL	n	Exponent in the Launder-Priddin modified mixing length formula for the inner region of the Baldwin-Lomax turbulence model. (TURB1)
* CONE	C_1	Constant used in the production term of the ε equation. (TURB20)
CP(I1,I2)	c_p	Specific heat at constant pressure at time level n . (FLOW1)
* CTHREE	C_3	Constant used to compute C_μ in the turbulent viscosity formula for the k - ε equations. (TURB20)
* CTWOR	C_{2r}	Constant used to compute C_2 in the dissipation term of the ε equation. (TURB20)
CV(I1,I2)	c_v	Specific heat at constant volume at time level n . (FLOW1)
* CVK	κ	Von Karman mixing length constant used in the inner region of the Baldwin-Lomax and Spalding-Kleinstein turbulence models. (TURB1)
* CWK	C_{wk}	Constant used in the formula for F_{wake} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
DEL	$\Delta\xi$ or $\Delta\eta$	Computational grid spacing in the ADI sweep direction. (NUM1)
DETA	$\Delta\eta$	Computational grid spacing in the η direction. (NUM1)
DPDET(I)	$\partial p / \partial E_T$	The derivative of p with respect to E_T , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DPDRHO(I)	$\partial p / \partial \rho$	The derivative of p with respect to ρ , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DPDRU(I)	$\partial p / \partial (\rho u)$	The derivative of p with respect to ρu , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)

DPDRV(I)	$\partial p / \partial(\rho v)$	The derivative of p with respect to ρv , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DPDRW(I)	$\partial p / \partial(\rho w)$	The derivative of p with respect to ρw , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
* DT(I)	Δt	The time step size, when specified directly as input. I is the time step sequence number, and runs from 1 to NTSEQ. (TIME1)
DTAU(I1,I2)	$\Delta \tau$	Computational time step size. (TIME1)
DTDET(I)	$\partial T / \partial E_T$	The derivative of T with respect to E_T , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DTDRHO(I)	$\partial T / \partial \rho$	The derivative of T with respect to ρ , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DTDRU(I)	$\partial T / \partial(\rho u)$	The derivative of T with respect to ρu , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DTDRV(I)	$\partial T / \partial(\rho v)$	The derivative of T with respect to ρv , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
DTDRW(I)	$\partial T / \partial(\rho w)$	The derivative of T with respect to ρw , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
* DTF1		Factor by which the time step is multiplied if the solution changes too slowly. (TIME1)
* DTF2		Factor by which the time step is divided if the solution changes too quickly. (TIME1)
* DTMAX		Maximum value that $\Delta \tau$ is allowed to reach, or the maximum $\Delta \tau$ used in the time step cycling procedure. (TIME1)
* DTMIN		Minimum value that $\Delta \tau$ is allowed to reach, or the minimum $\Delta \tau$ used in the time step cycling procedure. (TIME1)
DUMMY(I1,I2)		Dummy array used for temporary storage in several subroutines. (DUMMY1)
DXI	$\Delta \xi$	Computational grid spacing in the ξ direction. (NUM1)
E(I1,I2)	ε	Turbulent dissipation rate at time level n . (TURB20)
EL(I1,I2)	ε	Turbulent dissipation rate at previous or intermediate time level. (TURB20)
* EPS(I)	ε	Convergence level to be reached. The subscript I = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (TIME1)

ER	e_r	Dimensional reference energy, $\rho_r u_r^2$. (FLOW1)
ET(I1,I2)	E_T	Total energy at time level n . (FLOW1)
ETAT(I1,I2)	η_t	The derivative of the computational coordinate η with respect to untransformed time t . (METRIC1)
ETAX(I1,I2)	η_x	The derivative of the computational coordinate η with respect to the Cartesian coordinate x . (METRIC1)
ETAY(I1,I2)	η_y or η_r	The derivative of the computational coordinate η with respect to the Cartesian coordinate y or cylindrical coordinate r . (METRIC1)
ETL(I1,I2)	E_T	Total energy at previous or intermediate time level. (FLOW1)
* FBCT1(I2,I,J)		Point-by-point values used for boundary conditions for the k - ε turbulence model on the $\xi = 0$ and $\xi = 1$ boundaries. These are either set in the input, if a point-by-point distribution is being specified by the user, or by the program itself. The subscript $I = 1$ or 2 , corresponding to the k and ε equations, respectively, and $J = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC2)
* FBCT2(I1,I,J)		Point-by-point values used for boundary conditions for the k - ε turbulence model on the $\eta = 0$ and $\eta = 1$ boundaries. These are either set in the input, if a point-by-point distribution is being specified by the user, or by the program itself. The subscript $I = 1$ or 2 , corresponding to the k and ε equations, respectively, and $J = 1$ or 2 , corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC2)
* FBC1(I2,I,J)		Point-by-point values used for steady boundary conditions on the $\xi = 0$ and $\xi = 1$ surfaces. These are either set in the input, if a point-by-point distribution is being specified by the user, or by the program itself. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* FBC2(I1,I,J)		Point-by-point values used for steady boundary conditions on the $\eta = 0$ and $\eta = 1$ surfaces. These are either set in the input, if a point-by-point distribution is being specified by the user, or by the program itself. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
* GAMR	γ_r	Reference ratio of specific heats, c_{pr}/c_{vr} . (FLOW1)
* GBCT1(I,J)		Values used for boundary conditions for the k - ε turbulence model on the $\xi = 0$ and $\xi = 1$ boundaries, when specified for the entire surface. The subscript $I = 1$ or 2 , corresponding to the k and ε equations, respectively, and $J = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC2)
* GBCT2(I,J)		Values used for boundary conditions for the k - ε turbulence model on the $\eta = 0$ and $\eta = 1$ boundaries, when specified for the entire surface. The subscript $I = 1$ or 2 , corresponding to the k and ε equations, respectively, and $J = 1$ or 2 , corre-

		spending to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC2)
* GBC1(I,J)		Values used for steady boundary conditions on the $\xi = 0$ and $\xi = 1$ boundaries, when specified for the entire surface. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* GBC2(I,J)		Values used for steady boundary conditions on the $\eta = 0$ and $\eta = 1$ boundaries, when specified for the entire surface. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
GC	g_c	Dimensional proportionality factor in Newton's second law, either 32.174 lb _m -ft/lb _f -sec ² , or 1.0 kg-m/N-sec ² . (FLOW1)
* GTBC1(K,I,J)		A variable used to specify the values for unsteady and time-periodic boundary conditions on the $\xi = 0$ and $\xi = 1$ boundaries. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. For general unsteady boundary conditions, $K = 1$ to NTBC, corresponding to the time levels in the array NTBCA, and GTBC1 specifies the boundary condition value directly. For time-periodic boundary conditions, $K = 1$ to 4, and GTBC1 specifies the four coefficients in the equation used to determine the boundary condition value. (BC1)
* GTBC2(K,I,J)		A variable used to specify the values for unsteady and time-periodic boundary conditions on the $\eta = 0$ and $\eta = 1$ boundaries. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and $J = 1$ or 2 , corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. For general unsteady boundary conditions, $K = 1$ to NTBC, corresponding to the time levels in the array NTBCA, and GTBC2 specifies the boundary condition value directly. For time-periodic boundary conditions, $K = 1$ to 4, and GTBC2 specifies the four coefficients in the equation used to determine the boundary condition value. (BC1)
HSTAG	h_T	Stagnation enthalpy used with constant stagnation enthalpy option. (FLOW1)
* HSTAGR	$h_{T,r}$	Dimensional stagnation enthalpy used with constant stagnation enthalpy option. (FLOW1)
* IAV2E		Flag for second-order explicit artificial viscosity; 0 for none, 1 for constant coefficient model, 2 for nonlinear coefficient model. (NUM1)
* IAV2I		Flag for second-order implicit artificial viscosity; 0 for none, 1 for constant coefficient model. (NUM1)
* IAV4E		Flag for fourth-order explicit artificial viscosity; 0 for none, 1 for constant coefficient model, 2 for nonlinear coefficient model. (NUM1)

* IAXI	Flag for two-dimensional planar or axisymmetric flow; 0 for two-dimensional planar, 1 for axisymmetric. (GMTRY1)
IBASE	Base index used with ISTEP to compute one-dimensional index for two-dimensional array. Then, for example, for any sweep $U(I1,I2) = U1(IBASE + ISTEP*(I - 1))$ where I is the grid index in the sweep direction. (NUM1)
IBCELM(I,J)	Flags for elimination of off-diagonal sub-matrices resulting from gradient or extrapolation boundary conditions: 0 if elimination is not necessary, 1 if it is. The subscript I = 1 or 2 corresponding to the sweep direction, and J = 1 or 2 corresponding to the lower or upper boundary in that direction. (BC1)
* IBCT1(I2,I,J)	Flags specifying, point-by-point, the type of boundary conditions used for the k - ϵ turbulence model on the $\xi = 0$ and $\xi = 1$ surfaces. These are either set in the input, if a point-by-point distribution is specified by the user, or by the program itself. The subscript I = 1 or 2, corresponding to the k and ϵ equations, respectively, and J = 1 or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC2)
* IBCT2(I1,I,J)	Flags specifying, point-by-point, the type of boundary conditions used for the k - ϵ turbulence model on the $\eta = 0$ and $\eta = 1$ surfaces. These are either set in the input, if a point-by-point distribution is specified by the user, or by the program itself. The subscript I = 1 or 2, corresponding to the k and ϵ equations, respectively, and J = 1 or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC2)
* IBC1(I2,I,J)	Flags specifying, point-by-point, the type of steady boundary conditions used on the $\xi = 0$ and $\xi = 1$ surfaces. These are either set in the input, if a point-by-point distribution is specified by the user, or by the program itself. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* IBC2(I1,I,J)	Flags specifying, point-by-point, the type of steady boundary conditions used on the $\eta = 0$ and $\eta = 1$ surfaces. These are either set in the input, if a point-by-point distribution is specified by the user, or by the program itself. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
IBVUP(I)	Flags for updating boundary values from the first sweep after the last sweep: 0 if updating is not necessary, 1 if it is. Updating is required when gradient or extrapolation boundary conditions are used. The subscript I = 1 or 2, corresponding to the lower or upper boundary in the first sweep direction. (BC1)
* ICHECK	Results are checked for convergence every ICHECK'th time level. (TIME1)
ICONV	Convergence flag; 0 if not converged, 1 if converged. (TIME1)

* ICTEST	Flag for convergence criteria to be used. (TIME1)
* ICVARS	Parameter specifying which variables are being supplied as initial conditions by subroutine INIT. (FLOW1)
* IDEBUG(I)	A 20-element array of flags specifying various debug options. (IO1)
* IDTAU	Flag for time step selection method. (TIME1)
* IDTMOD	The time step size is modified every IDTMOD'th time step. (TIME1)
* IEULER	Flag for Euler calculation option; 0 for a full time-averaged Navier-Stokes calculation, 1 for an Euler calculation. (FLOW1)
IGAM	Flag set by method used to select GAMR; 0 if GAMR is defaulted (and hence c_p and c_v are functions of temperature), 1 if GAMR is specified by user (and hence c_p and c_v are constants). (FLOW1)
IGINT(I)	Flags for grid interpolation requirement; 0 if interpolation is not needed, 1 if interpolation is needed. The subscript $I = 1$ or 2 , corresponding to the ξ and η directions, respectively. (GMTRY1)
* IHSTAG	Flag for constant stagnation enthalpy option; 0 to solve the energy equation, 1 to eliminate the energy equation by assuming constant stagnation enthalpy. (FLOW1)
* ILAMV	Flag for computation of laminar viscosity and thermal conductivity; 0 for constant values, 1 for functions of local temperature. (FLOW1)
* ILDAMP	Flag for the Launder-Priddin modified mixing length formula in the inner region of the Baldwin-Lomax turbulence model. (TURB1)
INEG	Flag indicating non-positive values of pressure and/or temperature: 0 for no non-positive values, 1 for some. (FLOW1)
* INNER	Flag for type of inner region turbulence model. (TURB1)
* IPACK(I)	Flags for grid packing option; 0 for no packing, 1 to pack points as specified by the input array SQ. The subscript $I = 1$ or 2 , corresponding to the ξ and η directions, respectively. (NUM1)
* IPLOT	Flag controlling the creation of an auxiliary file, usually called a "plot file", used for later post-processing. (IO1)
* IPLT	Results are written into the plot file every IPLT time levels. (IO1)
* IPLTA(I)	Time levels at which results are written into the plot file. The subscript $I = 1$ to 101, the maximum number of time levels that may be written. (IO1)

* IPRT		Results are printed every IPRT time levels. (IO1)
* IPRTA(I)		Time levels at which results are printed. The subscript I = 1 to IO1, the maximum number of time levels that may be printed. (IO1)
* IPRT1		Results are printed at every IPRT1'th mesh point in the ξ direction. (IO1)
* IPRT2		Results are printed at every IPRT2'th mesh point in the η direction. (IO1)
* IPRT1A(I)		ξ indices at which results are printed. The subscript I = 1 to a maximum of N1, the number of grid points in the ξ direction. (IO1)
* IPRT2A(I)		η indices at which results are printed. The subscript I = 1 to a maximum of N2, the number of grid points in the η direction. (IO1)
* IREST		Flag controlling the reading and writing of auxiliary files used for restarting the calculation in a separate run. (RSTRT1)
ISTEP		Multiplication factor used with IBASE to compute one-dimensional index for two-dimensional array. (NUM1)
ISWEEP		Flag specifying ADI sweep direction; 1 for ξ direction and 2 for η direction. (NUM1)
* ISWIRL		Flag for swirl in axisymmetric flow; 0 for no swirl, 1 for swirl. (FLOW1)
IT	n	Current time step number, or known time level. Time step number n updates the solution from time level n to $n + 1$. (TIME1)
ITBEG		The time time step number, or known time level n , at the beginning of a run. For a non-restart case, ITBEG = 1. (TIME1)
ITDBC		Flag for time-dependent boundary conditions; 0 if all boundary conditions are steady, 1 if any general unsteady boundary conditions are used, 2 if only steady and time-periodic boundary conditions are used. (BC1)
ITEND		The final time step number. (TIME1)
* ITETA		Flag for computing turbulent viscosity on constant η lines. (TURB1)
* ITHIN(I)		Flags for thin-layer option; 0 to include 2nd. derivative viscous terms, 1 to eliminate them. The subscript I = 1 or 2, corresponding to the ξ and η directions, respectively. (FLOW1)
ITSEQ		Current time step sequence number. (TIME1)
* ITURB		Flag for turbulent flow option; 0 for laminar flow, 1 for turbulent flow using the Baldwin-Lomax algebraic turbulence

		model, 20 for turbulent flow using the Chien two-equation k - ϵ turbulence model. (TURB1)
* ITXI		Flag for computing turbulent viscosity on constant ξ lines. (TURB1)
* IUNITS		Flag for type of units used to specify reference conditions; 0 for English units, 1 for SI units. (IO1)
IV	i	Grid point index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized). Therefore, $IV = j$ for the first sweep and i for the second sweep. (NUM1)
* IVOUT(I)		A 50-element array specifying which variables are to be printed. (IO1)
* IWALL1(I)		Flags indicating type of surfaces in the ξ direction; 0 for a free boundary, 1 for a solid wall. The subscript $I = 1$ or 2, corresponding to the $\xi = 0$ and $\xi = 1$ surfaces, respectively. (TURB1)
* IWALL2(I)		Flags indicating type of surfaces in the η direction; 0 for a free boundary, 1 for a solid wall. The subscript $I = 1$ or 2, corresponding to the $\eta = 0$ and $\eta = 1$ surfaces, respectively. (TURB1)
* IWOUT1(I)		Flags specifying whether or not various parameters are to be printed along the ξ boundaries; 0 for no printout, 1 for printout along the boundary. The subscript $I = 1$ or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (IO1)
* IWOUT2(I)		Flags specifying whether or not various parameters are to be printed along the η boundaries; 0 for no printout, 1 for printout along the boundary. The subscript $I = 1$ or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (IO1)
I1	i	Grid point index in the ξ direction. (NUM1)
I2	j	Grid point index in the η direction. (NUM1)
* JBCT1(I,J)		Flags specifying the type of boundary conditions used for the k - ϵ turbulence model on the $\xi = 0$ and $\xi = 1$ surfaces, when specified for the entire surface. The subscript $I = 1$ or 2, corresponding to the k and ϵ equations, respectively, and $J = 1$ or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC2)
* JBCT2(I,J)		Flags specifying the type of boundary conditions used for the k - ϵ turbulence model on the $\eta = 0$ and $\eta = 1$ surfaces, when specified for the entire surface. The subscript $I = 1$ or 2, corresponding to the k and ϵ equations, respectively, and $J = 1$ or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC2)
* JBC1(I,J)		Flags specifying the type of steady boundary conditions used on the $\xi = 0$ and $\xi = 1$ surfaces, when specified for the entire

		surface. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* JBC2(I,J)		Flags specifying the type of steady boundary conditions used on the $\eta = 0$ and $\eta = 1$ surfaces, when specified for the entire surface. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
JI(I1,I2)	J^{-1} or rJ^{-1}	Normally the inverse Jacobian of the non-orthogonal grid transformation. For the COEF routines in axisymmetric flow, it is temporarily redefined as the product of the local radius and the inverse Jacobian. This is a real variable. (METRIC1)
* JTBC1(I,J)		A variable specifying the type of time dependency for the boundary conditions on the $\xi = 0$ and $\xi = 1$ boundaries. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* JTBC2(I,J)		A variable specifying the type of time dependency for the boundary conditions on the $\eta = 0$ and $\eta = 1$ boundaries. I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
KBCPER(I)		Flags for spatially periodic boundary conditions: 0 for non-periodic, 1 for periodic. The subscript I = 1 or 2, corresponding to the ξ and η directions, respectively. (BC1)
* KBC1(J)		Flags for type of boundaries in the ξ direction. The subscript J = 1 or 2, corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (BC1)
* KBC2(J)		Flags for type of boundaries in the η direction. The subscript J = 1 or 2, corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (BC1)
KE(I1,I2)	k	Turbulent kinetic energy at time level n . This is a real variable. (TURB20)
KEL(I1,I2)	k	Turbulent kinetic energy at previous or intermediate time level. This is a real variable. (TURB20)
KT(I1,I2)	k	Effective thermal conductivity coefficient at time level n . This is a real variable. (FLOW1)
* KTR	k_r	Dimensional reference thermal conductivity coefficient. This is a real variable. (FLOW1)
LA(I1,I2)	λ	Effective second coefficient of viscosity at time level n (usually assumed equal to $-2\mu/3$.) This is a real variable. (FLOW1)
* LR	L_r	Dimensional reference length. This is a real variable. (FLOW1)

LRMAX(I,J,K)		The grid indices corresponding to the location of the maximum absolute value of the residual. The subscript $I = 1$ or 2 , corresponding to the ξ and η directions, respectively, $J = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations, and $K = 1$ or 2 , corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
LWAKE1(I2)		Grid point index in the ξ direction used as the origin for computing length scales for free turbulent flows. (TURB1)
LWAKE2(I1)		Grid point index in the η direction used as the origin for computing length scales for free turbulent flows. (TURB1)
* LWALL1(I2,I)		Flags indicating, point-by-point, the type of surfaces in the ξ direction; 0 for a free boundary, 1 for a solid wall. The subscript $I = 1$ or 2 , corresponding to the $\xi = 0$ and $\xi = 1$ boundaries, respectively. (TURB1)
* LWALL2(I1,I)		Flags indicating, point-by-point, the type of surfaces in the η direction; 0 for a free boundary, 1 for a solid wall. The subscript $I = 1$ or 2 , corresponding to the $\eta = 0$ and $\eta = 1$ boundaries, respectively. (TURB1)
LWSET(I)		Flags specifying how wall locations are determined for the turbulence model; 0 if wall locations are found automatically by searching for boundary points where the velocity is zero, 1 if input using the LWALL parameters, 2 if input using the IWALL parameters. The subscript $I = 1$ to 4 , corresponding to the $\xi = 0$, $\xi = 1$, $\eta = 0$, and $\eta = 1$ boundaries, respectively. (TURB1)
* MACHR	M_r	Reference Mach number, $u_r/(\gamma \bar{R} T_r)^{1/2}$. This is a real variable. (FLOW1)
METT1(I)	ξ_t or η_t	The derivative of the computational coordinate in the ADI sweep direction with respect to untransformed time t . In actual use, this one-dimensional array is equivalenced to the two-dimensional array METT(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_s - 1$. This is a real variable. (METRIC1)
METX1(I)	ξ_x or η_x	The derivative of the computational coordinate in the ADI sweep direction with respect to the Cartesian coordinate x . In actual use, this one-dimensional array is equivalenced to the two-dimensional array METX(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_s - 1$. This is a real variable. (METRIC1)
METY1(I)	ξ_y or η_y	The derivative of the computational coordinate in the ADI sweep direction with respect to the Cartesian coordinate y or cylindrical coordinate r . In actual use, this one-dimensional array is equivalenced to the two-dimensional array METY(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK"

			routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
	MU(I1,I2)	μ	Effective viscosity coefficient at time level n . This is a real variable. (FLOW1)
*	MUR	μ_r	Dimensional reference viscosity coefficient. This is a real variable. (FLOW1)
	MUT(I1,I2)	μ_t	Turbulent viscosity coefficient at time level n . This is a real variable. (FLOW1)
	MUTL(I1,I2)	μ_t	Turbulent viscosity coefficient at previous or intermediate time level. This is a real variable. (TURB20)
	NAMAX		A dimensioning parameter equal to the maximum number of time steps allowed in the moving average convergence test (the ICTEST = 2 option). (PARAMS1)
	NBC		A dimensioning parameter equal to the number of boundary conditions per equation. (PARAMS1)
	NC		Array index associated with the continuity equation. (NUM1)
*	NDTCYC		Number of time steps per cycle used in the time step cycling procedure. (TIME1)
	NEN		Array index associated with the energy equation. (NUM1)
	NEQ	N_{eq}	The number of coupled governing equations actually being solved. (NUM1)
	NEQP		A dimensioning parameter equal to the number of coupled equations allowed. (PARAMS1)
	NEQPM		A dimensioning parameter equal to the maximum number of coupled equations available. (PARAMS1)
	NET		Array index associated with the dependent variable E_T . (NUM1)
*	NGEOM		Flag used to specify type of computational coordinates; 1 for Cartesian (x,y) coordinates, 2 for polar (r',θ') coordinates, and 10 to read the coordinates from unit NGRID. (GMTRY1)
*	NGRID		Unit number for reading grid file. (IO1)
*	NHIST		Unit number for writing convergence history file. (IO1)
*	NHMAX		Maximum number of time levels allowed in the printout of the convergence history file (not counting the first two, which are always printed.) (IO1)
	NIN		Unit number for reading namelist input. (IO1)
*	NITAVG		Number of time steps used in the moving average convergence test. (TIME1)

NMAXP		A dimensioning parameter equal to the maximum of N1P and N2P. (PARAMS1)
* NOUT		Unit number for writing standard output. (IO1)
* NPLOT		Unit number for writing CONTOUR or PLOT3D Q plot file. (IO1)
* NPLOTX		Unit number for writing PLOT3D XYZ plot file. (IO1)
NPRT1		Total number of indices for printout in the ξ direction. (IO1)
NPRT2		Total number of indices for printout in the η direction. (IO1)
NPTS	N	The number of grid points in the sweep direction. (NUM1)
NPT1	N_1 or $N_1 + 1$	The number of grid points in the ξ direction used in computing coefficients: N_1 for non-periodic boundary conditions; $N_1 + 1$ for spatially periodic boundary conditions. (NUM1)
NPT2	N_2 or $N_2 + 1$	The number of grid points in the η direction used in computing coefficients: N_2 for non-periodic boundary conditions; $N_2 + 1$ for spatially periodic boundary conditions. (NUM1)
NR		Array index associated with the dependent variable ρ . (NUM1)
* NRQIN		Unit number for reading restart flow field. (RSTRT1)
* NRQOUT		Unit number for writing restart flow field. (RSTRT1)
NRU		Array index associated with the dependent variable ρu . (NUM1)
NRV		Array index associated with the dependent variable ρv . (NUM1)
NRW		Array index associated with the dependent variable ρw . (NUM1)
* NRXIN		Unit number for reading restart computational mesh. (RSTRT1)
* NRXOUT		Unit number for writing restart computational mesh. (RSTRT1)
* NSCR1		Unit number for scratch file in subroutine PLOT. (IO1)
* NTBC		Number of values in the tables of GTBC1 and/or GTBC2 vs. NTBCA for general unsteady boundary conditions. (BC1)
* NTBCA(I)		Time levels at which GTBC1 and/or GTBC2 are specified for general unsteady boundary conditions. The subscript $I = 1$ to NTBC, corresponding to the NTBC values in the table. (BC1)
* NTIME(I)		Maximum number of time steps to march. I runs from 1 to NTSEQP, corresponding to the time step sequence number. (TIME1)

* NTKE		Number of k - ϵ iterations per mean flow iteration. (TURB20)
NTOTP		A dimensioning parameter equal to the total storage required for a single two-dimensional array (i.e., $N1P \times N2P$). (PARAMS1)
NTP		A dimensioning parameter equal to the maximum number of entries in the table of time-dependent boundary condition values. (PARAMS1)
* NTSEQ		The total number of time step sequences being used. (TIME1)
NTSEQP		A dimensioning parameter equal to the maximum number of time step sequences in the time step sequencing option. (PARAMS1)
NV	N_v	The number of grid points in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized). Therefore, $NV = N_2$ for the first sweep and N_1 for the second sweep. (NUM1)
NXM		Array index associated with the x -momentum equation. (NUM1)
NYM		Array index associated with the y or r -momentum equation. (NUM1)
NZM		Array index associated with the swirl momentum equation. (NUM1)
* N1	N_1	The number of grid points in the ξ direction. (NUM1)
N1P		A dimensioning parameter equal to the maximum number of grid points in the ξ direction. (PARAMS1)
* N2	N_2	The number of grid points in the η direction. (NUM1)
N2P		A dimensioning parameter equal to the maximum number of grid points in the η direction. (PARAMS1)
P(I1,I2)	p	Static pressure at time level n . (FLOW1)
PONE	P_1	Part 1 of the production rate of the turbulent kinetic energy. (TURB20)
PR	p_r	Dimensional reference static pressure, $\rho_r \bar{R} T_r / g_c$. (FLOW1)
* PRLR	Pr_{lr}	Reference laminar Prandtl number, $c_{p,r} \mu_r / k_r$, where $c_{p,r} = \gamma_r \bar{R} / (\gamma_r - 1)$. (FLOW1)
PRR	Pr_r	Reference Prandtl number, $\mu_r u_r^2 / k_r T_r$. (FLOW1)
* PRT	Pr_t	Turbulent Prandtl number, or, if non-positive, a flag indicating the use of a variable turbulent Prandtl number. (TURB1)
PTWO	P_2	Part 2 of the production rate of the turbulent kinetic energy. (TURB20)

* P0	p_0	Initial static pressure. (IC1)
RAX(I)	1 or r	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow. I is the grid index in the sweep direction, running from 1 to N . (METRIC1)
* RER	Re_r	Reference Reynolds number, $\rho_r u_r L_r / \mu_r$. (FLOW1)
RESAVG(J,K)	R_{avg}	The average absolute value of the residual for the previous time step. The subscript $J = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations, and $K = 1$ or 2 , corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
RESL2(J,K)	R_{L_2}	The L_2 norm of the residual for the previous time step. The subscript $J = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations, and $K = 1$ or 2 , corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
RESMAX(J,K)	R_{max}	The maximum absolute value of the residual for the previous time step. The subscript $J = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations, and $K = 1$ or 2 , corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
* REXT1	$Re_{x_{tr}}$	Reynolds number at the beginning of the transition region, based on maximum total velocity and distance from $\xi = 0$, for flow predominantly in the ξ direction with a leading edge at $\xi = 0$. (TURB1)
* REXT2	$Re_{\eta_{tr}}$	Reynolds number at the beginning of the transition region, based on maximum total velocity and distance from $\eta = 0$, for flow predominantly in the η direction with a leading edge at $\eta = 0$. (TURB1)
* RG	\bar{R}	Dimensional gas constant. (FLOW1)
RGAS	R	Nondimensional gas constant. (FLOW1)
RHO(I1,I2)	ρ	Static density at time level n . (FLOW1)
RHOL(I1,I2)	ρ	Static density at previous or intermediate time level. (FLOW1)
* RHOR	ρ_r	Dimensional reference density. (FLOW1)
* RMAX	r'_{max}	Maximum r' coordinate for polar grid option. (GMTRY1)
* RMIN	r'_{min}	Minimum r' coordinate for polar grid option. (GMTRY1)
S	S	See SVECT1. (NUM1)
* SIGE	σ_ϵ	Constant used in the diffusion term of the ϵ equation. (TURB20)
* SIGK	σ_k	Constant used in the diffusion term of the k equation. (TURB20)

* SQ(I,J)		An array controlling the packing of grid points using the Roberts transformation. The subscript I = 1 or 2, corresponding to the ξ and η directions, respectively. SQ(I,1) specifies the location of packing, and SQ(I,2) specifies the amount of packing. (NUM1)
SVECT1(I)	S	Subvector of source terms in the block tridiagonal system of equations. In actual use, this one-dimensional array is equivalent to the three-dimensional array S(IV,IS,J). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
T(I1,I2)	T	Static temperature at time level n . (FLOW1)
TAU(I1,I2)	τ	Current value of the time marching parameter. (TIME1)
* TFACT		Factor used in computing the k - ϵ time step, $\Delta\tau_{k-\epsilon} = TFACT(\Delta\tau)$. (TURB20)
* THC(I)	θ_1, θ_2	A two-element array specifying the time difference centering parameters used for the continuity equation. (NUM1)
* THE(I)	$\theta_1, \theta_2, \theta_3$	A three-element array specifying the time difference centering parameters used for the energy equation. (NUM1)
* THKE(I)	θ_1, θ_2	A two-element array specifying the time difference centering parameters used for the k - ϵ equations. (NUM2)
* THMAX	θ'_{max}	Maximum θ' coordinate in degrees for polar grid option. (GMTRY1)
* THMIN	θ'_{min}	Minimum θ' coordinate in degrees for polar grid option. (GMTRY1)
* THX(I)	$\theta_1, \theta_2, \theta_3$	A three-element array specifying the time difference centering parameters used for the x -momentum equation. (NUM1)
* THY(I)	$\theta_1, \theta_2, \theta_3$	A three-element array specifying the time difference centering parameters used for the y or r -momentum equation. (NUM1)
* THZ(I)	$\theta_1, \theta_2, \theta_3$	A three-element array specifying the time difference centering parameters used for the swirl momentum equation. (NUM1)
* TITLE		Title for printed output and CONTOUR plot file, up to 72 characters long. This is a character variable. (TITLE1)
TL(I1,I2)	T	Static temperature at previous or intermediate time level. (FLOW1)
* TLIM		When the amount of CPU time remaining for the job drops below TLIM seconds, the calculation is stopped. (TIME1)
* TR	T_r	Dimensional reference temperature. (FLOW1)
* T0	T_0	Initial static temperature. (IC1)

U(I1,I2)	u	Velocity in the Cartesian x direction at time level n . (FLOW1)
UL(I1,I2)	u	Velocity in the Cartesian x direction at previous or intermediate time level. (FLOW1)
* UR	u_r	Dimensional reference velocity. (FLOW1)
* U0	u_0	Initial velocity in the Cartesian x direction. (IC1)
V(I1,I2)	v	Velocity in the Cartesian y direction or cylindrical r direction at time level n . (FLOW1)
VL(I1,I2)	v	Velocity in the Cartesian y direction or cylindrical r direction at previous or intermediate time level. (FLOW1)
VORT(I1,I2)	$ \bar{\Omega} $	Total vorticity magnitude. (TURB1)
VORT(I1,I2)	$ \bar{\Omega} $	Production rate of turbulent kinetic energy. (TURB1)
* V0	v_0	Initial velocity in the Cartesian y direction or cylindrical r direction. (IC1)
W(I1,I2)	w	Swirl velocity at time level n . (FLOW1)
WL(I1,I2)	w	Swirl velocity at previous or intermediate time level. (FLOW1)
* W0	w_0	Initial swirl velocity. (IC1)
X(I1,I2)	x	Cartesian x coordinate. (METRIC1)
XIT(I1,I2)	ξ_r	The derivative of the computational coordinate ξ with respect to untransformed time t . (METRIC1)
XIX(I1,I2)	ξ_x	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate x . (METRIC1)
XIY(I1,I2)	ξ_y or ξ_r	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate y or cylindrical coordinate r . (METRIC1)
* XMAX	x_{max}	Maximum x coordinate for Cartesian grid option. (GMTRY1)
* XMIN	x_{min}	Minimum x coordinate for Cartesian grid option. (GMTRY1)
Y(I1,I2)	y or r	Cartesian y coordinate or cylindrical r coordinate. (METRIC1)
* YMAX	y_{max}	Maximum y coordinate for Cartesian grid option. (GMTRY1)
* YMIN	y_{min}	Minimum y coordinate for Cartesian grid option. (GMTRY1)

YPLUSD(I1,I2)	y^+	Non-dimensional distance from the nearest solid wall. (TURB20)
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3.3 COMMON VARIABLES LISTED SYMBOLICALLY

In this section many of the *Proteus* Fortran variables stored in common blocks are defined, listed symbolically. Note that this list does not include those variables without symbolic representations, such as various flags, or those whose meaning depends on other parameters, such as the boundary condition values and sweep direction metrics. The variables marked with an asterisk are input variables. More details on these may be found in Section 3.1 of Volume 2. The common block each variable is stored in is given in parentheses at the end of each definition. For subscripted variables, the subscripts are defined along with the variable, except for the subscripts I1 and I2, which are the indices i and j in the ξ and η directions, respectively, and run from 1 to N_1 and N_2 .

Unless otherwise noted, all variables representing physical quantities are nondimensional. The nondimensionalizing procedure is described in Section 3.1.1 of Volume 2. The type (real or integer) of the variables follows standard Fortran convention, unless stated otherwise. (I.e., those starting with I, J, K, L, M, or N are integer, and the remainder are real.)

<u>Symbol</u>	<u>Fortran Variable</u>	<u>Definition</u>
* A^+	APLUS	Van Driest damping constant in the inner and outer regions of the Baldwin-Lomax turbulence model. (TURB1)
A	AMAT1(I)	Subdiagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array A(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)
* B	CB	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbulence model, and in the inner region of the Spalding-Kleinstein turbulence model. (TURB1)
B	BMAT1(I)	Diagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array B(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)
c_p	CP(I1,I2)	Specific heat at constant pressure at time level n . (FLOW1)
c_v	CV(I1,I2)	Specific heat at constant volume at time level n . (FLOW1)
* C_{cp}	CCP	Constant used in the outer region of the Baldwin-Lomax turbulence model. (TURB1)

$C_{cp1} - C_{cp4}$	CCP1-CCP4	Constants in empirical formula for specific heat as a function of temperature. (FLOW1)
$C_{k1} - C_{k2}$	CK1-2	Constants in empirical formula for thermal conductivity coefficient as a function of temperature.
* C_{Kleb}	CKLEB	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* $(C_{Kleb})_{min}$	CKMIN	Constant used in the formula for the Klebanoff intermittency factor F_{Kleb} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* $C_{\mu r}$	CMUR	Constant used to compute C_μ in the turbulent viscosity formula for the $k-\epsilon$ equations. (TURB20)
$C_{\mu 1} - C_{\mu 2}$	CMU1-2	Constants in empirical formula for laminar viscosity coefficient as a function of temperature. (FLOW1)
* C_{wk}	CWK	Constant used in the formula for F_{wake} in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* C_1	CONE	Constant used in the production term of the ϵ equation. (TURB20)
* C_{2r}	CTWOR	Constant used to compute C_2 in the dissipation term of the ϵ equation. (TURB20)
* C_3	CTHREE	Constant used to compute C_μ in the turbulent viscosity formula for the $k-\epsilon$ equations. (TURB20)
C	CMAT1(I)	Superdiagonal submatrix of coefficients in the block tridiagonal coefficient matrix. In actual use, this one-dimensional array is equivalenced to the four-dimensional array C(IV,IS,J,K). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (NUM1)
e_r	ER	Dimensional reference energy, ρu^2 . (FLOW1)
E_T	ET(I1,I2)	Total energy at time level n . (FLOW1)
E_T	ETL(I1,I2)	Total energy at previous or intermediate time level. (FLOW1)
g_c	GC	Dimensional proportionality factor in Newton's second law, either 32.174 lb _m -ft/lb _f -sec ² , or 1.0 kg-m/N-sec ² . (FLOW1)
h_T	HSTAG	Stagnation enthalpy used with constant stagnation enthalpy option. (FLOW1)
* h_{Tr}	HSTAGR	Dimensional stagnation enthalpy used with constant stagnation enthalpy option. (FLOW1)
i	I1	Grid point index in the ξ direction. (NUM1)

i	IV	Grid point index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized). Therefore, IV = j for the first sweep and i for the second sweep. (NUM1)
j	I2	Grid point index in the η direction. (NUM1)
J^{-1}	JI(I1,I2)	Inverse Jacobian of the non-orthogonal grid transformation. (For axisymmetric flow, in the COEF routines $JI = rJ^{-1}$, the product of the local radius and the inverse Jacobian.) This is a real variable. (METRIC1)
k	KT(I1,I2)	Effective thermal conductivity coefficient at time level n . This is a real variable. (FLOW1)
k	KE(I1,I2)	Turbulent kinetic energy at time level n . This is a real variable. (TURB20)
k	KEL(I1,I2)	Turbulent kinetic energy at previous or intermediate time level. This is a real variable. (TURB20)
* k_r	KTR	Dimensional reference thermal conductivity coefficient. This is a real variable. (FLOW1)
* K	CCLAU	Clauser constant used in the outer region of the Baldwin-Lomax turbulence model. (TURB1)
* L_r	LR	Dimensional reference length. This is a real variable. (FLOW1)
* M_r	MACHR	Reference Mach number, $u_r/(\gamma_r \bar{R} T_r)^{1/2}$. This is a real variable. (FLOW1)
n	IT	Current time step number, or known time level. Time step number n updates the solution from time level n to $n + 1$. (TIME1)
* n	CNA	Exponent in the formula used to average the two outer region μ_r profiles that result when both boundaries in a coordinate direction are solid surfaces. (TURB1)
* n	CNL	Exponent in the Launder-Priddin modified mixing length formula for the inner region of the Baldwin-Lomax turbulence model. (TURB1)
N	NPTS	The number of grid points in the sweep direction. (NUM1)
N_{eq}	NEQ	The number of coupled governing equations actually being solved. (NUM1)
N_v	NV	The number of grid points in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized). Therefore, NV = N_2 for the first sweep and N_1 for the second sweep. (NUM1)
* N_1	N1	The number of grid points in the ξ direction. (NUM1)

N_1	NPT1	The number of grid points in the ξ direction used in computing coefficients (only for non-periodic boundary conditions.) (NUM1)
$N_1 + 1$	NPT1	The number of grid points in the ξ direction used in computing coefficients (only for spatially periodic boundary conditions.) (NUM1)
* N_2	N2	The number of grid points in the η direction. (NUM1)
N_2	NPT2	The number of grid points in the η direction used in computing coefficients (only for non-periodic boundary conditions.) (NUM1)
$N_2 + 1$	NPT2	The number of grid points in the η direction used in computing coefficients (only for spatially periodic boundary conditions.) (NUM1)
p	P(I1,I2)	Static pressure at time level n . (FLOW1)
p_r	PR	Dimensional reference static pressure, $\rho_r \bar{R} T_r / g_c$. (FLOW1)
* p_0	P0	Initial static pressure. (IC1)
$\partial p / \partial E_T$	DPDET(I)	The derivative of p with respect to E_T , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial p / \partial \rho$	DPDRHO(I)	The derivative of p with respect to ρ , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial p / \partial (\rho u)$	DPDRU(I)	The derivative of p with respect to ρu , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial p / \partial (\rho v)$	DPDRV(I)	The derivative of p with respect to ρv , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial p / \partial (\rho w)$	DPDRW(I)	The derivative of p with respect to ρw , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
P_1	PONE	Part 1 of the production rate of the turbulent kinetic energy. (TURB20)
P_2	PTWO	Part 2 of the production rate of the turbulent kinetic energy. (TURB20)
* Pr_r	PRLR	Reference laminar Prandtl number, $c_{p,r} \mu_r / k_r$, where $c_{p,r} = \gamma_r \bar{R} / (\gamma_r - 1)$. (FLOW1)
Pr_r	PRR	Reference Prandtl number, $\mu_r u_r^2 / k_r T_r$. (FLOW1)

* Pr_t	PRT	Turbulent Prandtl number, or, if non-positive, a flag indicating the use of a variable turbulent Prandtl number. (TURB1)
ΔQ_{avg}	CHGAVG(I)	Maximum change in absolute value of the dependent variables, averaged over the last NITAVG time steps. ⁶ The subscript I = 1 to N_{eq} , corresponding to the N_{eq} dependent variables. (TIME1)
ΔQ_{max}	CHGMAX(I,J)	Maximum change in absolute value of the dependent variables over a single time step. ⁶ The subscript I = 1 to N_{eq} , corresponding to the N_{eq} dependent variables, and J = 1 to NITAVG, the number of time steps used in the moving average option for determining convergence. (TIME1)
r	Y(I1,I2)	Cylindrical r coordinate. (METRIC1)
r	RAX(I)	Local radius r for axisymmetric flow. I is the grid index in the sweep direction, running from 1 to N . (METRIC1)
* r'_{max}	RMAX	Maximum r' coordinate coordinate for polar grid option. (GMTRY1)
* r'_{min}	RMIN	Minimum r' coordinate coordinate for polar grid option. (GMTRY1)
R_{avg}	RESAVG(J,K)	The average absolute value of the residual for the previous time step. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 or 2, corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
R_{L_2}	RESL2(J,K)	The L_2 norm of the residual for the previous time step. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 or 2, corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
R_{max}	RESMAX(J,K)	The maximum absolute value of the residual for the previous time step. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations, and K = 1 or 2, corresponding to the residual computed without and with the artificial viscosity terms. (TIME1)
* \bar{R}	RG	Dimensional gas constant. (FLOW1)
R	RGAS	Nondimensional gas constant. (FLOW1)
* Re_r	RER	Reference Reynolds number, $\rho_r u_r L_r / \mu_r$. (FLOW1)
* Re_{xtr}	REXT1	Reynolds number at the beginning of the transition region, based on maximum total velocity and distance from $\xi = 0$, for flow predominantly in the ξ direction with a leading edge at $\xi = 0$. (TURB1)

⁶ For the energy equation, the change in E_T is divided by $E_T = \rho_r \bar{R} T_r / (\gamma_r - 1) + u^2/2$, so that it is the same order of magnitude as the other conservation variables.

* Re_{xtr}	REXT2	Reynolds number at the beginning of the transition region, based on maximum total velocity and distance from $\eta = 0$, for flow predominantly in the η direction with a leading edge at $\eta = 0$. (TURB1)
S	SVECT1(I)	Subvector of source terms in the block tridiagonal system of equations. In actual use, this one-dimensional array is equivalent to the three-dimensional array S(IV,IS,J). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. The subscript J = 1 to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* Δt	DT(I)	The time step size, when specified directly as input. I is the time step sequence number, and runs from 1 to NTSEQ. (TIME1)
T	T(I1,I2)	Static temperature at time level n . (FLOW1)
T	TL(I1,I2)	Static temperature at previous or intermediate time level. (FLOW1)
$\partial T / \partial E_T$	DTDET(I)	The derivative of T with respect to E_T , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial T / \partial \rho$	DTDRHO(I)	The derivative of T with respect to ρ , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial T / \partial (\rho u)$	DTDRU(I)	The derivative of T with respect to ρu , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial T / \partial (\rho v)$	DTDRV(I)	The derivative of T with respect to ρv , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
$\partial T / \partial (\rho w)$	DTDRW(I)	The derivative of T with respect to ρw , stored as a one-dimensional array in the sweep direction. The subscript I therefore runs from 1 to N . (FLOW1)
* T_r	TR	Dimensional reference temperature. (FLOW1)
* T_0	T0	Initial static temperature. (IC1)
u	U(I1,I2)	Velocity in the Cartesian x direction at time level n . (FLOW1)
u	UL(I1,I2)	Velocity in the Cartesian x direction at previous or intermediate time level. (FLOW1)
* u_r	UR	Dimensional reference velocity. (FLOW1)
* u_0	U0	Initial velocity in the Cartesian x direction. (IC1)
v	V(I1,I2)	Velocity in the Cartesian y direction or cylindrical r direction at time level n . (FLOW1)

v	VL(I1,I2)	Velocity in the Cartesian y direction or cylindrical r direction at previous or intermediate time level. (FLOW1)
* v_0	V0	Initial velocity in the Cartesian y direction or cylindrical r direction. (IC1)
w	W(I1,I2)	Swirl velocity at time level n . (FLOW1)
w	WL(I1,I2)	Swirl velocity at previous or intermediate time level. (FLOW1)
* w_0	W0	Initial swirl velocity. (IC1)
x	X(I1,I2)	Cartesian x coordinate. (METRIC1)
* x_{max}	XMAX	Maximum x coordinate for Cartesian grid option. (GMTRY1)
* x_{min}	XMIN	Minimum x coordinate for Cartesian grid option. (GMTRY1)
y	Y(I1,I2)	Cartesian y coordinate. (METRIC1)
* y_{max}	YMAX	Maximum y coordinate for Cartesian grid option. (GMTRY1)
* y_{min}	YMIN	Minimum y coordinate for Cartesian grid option. (GMTRY1)
y^+	YPLUSD(I1,I2)	Non-dimensional distance from the nearest solid wall. (TURB20)
* ε	EPS(I)	Convergence level to be reached. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} dependent variables. (TIME1)
ε	E(I1,I2)	Turbulent dissipation rate at time level n . (TURB20)
ε	EL(I1,I2)	Turbulent dissipation rate at previous or intermediate time level. (TURB20)
* $\varepsilon_E^{(2)}$	CAVS2E(I)	Second-order explicit artificial viscosity coefficient in constant coefficient model. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* $\varepsilon_E^{(4)}$	CAVS4E(I)	Fourth-order explicit artificial viscosity coefficient in constant coefficient model. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* ε_I	CAVS2I(I)	Second-order implicit artificial viscosity coefficient in constant coefficient model. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
η_r	ETAY(I1,I2)	The derivative of the computational coordinate η with respect to the cylindrical coordinate r . (METRIC1)
η_r	METY1(I)	The derivative of the computational coordinate η with respect to the cylindrical coordinate r (second ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the

		two-dimensional array METY(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
η_t	ETAT(I1,I2)	The derivative of the computational coordinate η with respect to untransformed time t . (METRIC1)
η_t	METT1(I)	The derivative of the computational coordinate η with respect to untransformed time t (second ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METT(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
η_x	ETAX(I1,I2)	The derivative of the computational coordinate η with respect to the Cartesian coordinate x . (METRIC1)
η_x	METX1(I)	The derivative of the computational coordinate η with respect to the Cartesian coordinate x (second ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METX(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
η_y	ETAY(I1,I2)	The derivative of the computational coordinate η with respect to the Cartesian coordinate y . (METRIC1)
η_y	METY1(I)	The derivative of the computational coordinate η with respect to the Cartesian coordinate y (second ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METY(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
$\Delta\eta$	DEL	Computational grid spacing in the η direction (second ADI sweep only.) (NUM1)
$\Delta\eta$	DETA	Computational grid spacing in the η direction. (NUM1)
* κ	CVK	Von Karman mixing length constant used in the inner region of the Baldwin-Lomax and Spalding-Kleinstein turbulence models. (TURB1)
* κ_2	CAVS2E(I)	User-specified constant in nonlinear coefficient artificial viscosity model. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)
* κ_4	CAVS4E(I)	User-specified constant in nonlinear coefficient artificial viscosity model. The subscript $I = 1$ to N_{eq} , corresponding to the N_{eq} coupled governing equations. (NUM1)

* γ_r	GAMR	Reference ratio of specific heats, $c_{p,r}/c_{v,r}$. (FLOW1)
λ	LA(I1,I2)	Effective second coefficient of viscosity at time level n (usually assumed equal to $-2\mu/3$.) This is a real variable. (FLOW1)
μ	MU(I1,I2)	Effective viscosity coefficient at time level n . This is a real variable. (FLOW1)
* μ_r	MUR	Dimensional reference viscosity coefficient. This is a real variable. (FLOW1)
μ_t	MUT(I1,I2)	Turbulent viscosity coefficient at time level n . This is a real variable. (FLOW1)
μ_t	MUTL(I1,I2)	Turbulent viscosity coefficient at previous or intermediate time level. This is a real variable. (TURB20)
ξ_r	XIY(I1,I2)	The derivative of the computational coordinate ξ with respect to the cylindrical coordinate r . (METRIC1)
ξ_r	METY1(I)	The derivative of the computational coordinate ξ with respect to the cylindrical coordinate r (first ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METY(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
ξ_t	XIT(I1,I2)	The derivative of the computational coordinate ξ with respect to untransformed time t . (METRIC1)
ξ_t	METT1(I)	The derivative of the computational coordinate ξ with respect to untransformed time t (first ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METT(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
ξ_x	XIX(I1,I2)	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate x . (METRIC1)
ξ_x	METX1(I)	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate x (first ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the two-dimensional array METX(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)
ξ_y	XIY(I1,I2)	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate y . (METRIC1)
ξ_y	METY1(I)	The derivative of the computational coordinate ξ with respect to the Cartesian coordinate y (first ADI sweep only.) In actual use, this one-dimensional array is equivalenced to the

two-dimensional array METY(IV,IS). IS is the grid index in the sweep direction, running from 1 to N . IV is the grid index in the "vectorized" direction (i.e., the non-sweep direction in which the "BLK" routines are vectorized), and runs from 2 to $N_v - 1$. This is a real variable. (METRIC1)

$\Delta \xi$	DEL	Computational grid spacing in the ξ direction (first ADI sweep only.) (NUM1)
$\Delta \xi$	DXI	Computational grid spacing in the ξ direction. (NUM1)
ρ	RHO(I1,I2)	Static density at time level n . (FLOW1)
ρ	RHOL(I1,I2)	Static density at previous or intermediate time level. (FLOW1)
* ρ_r	RHOR	Dimensional reference density. (FLOW1)
* σ_k	SIGK	Constant used in the diffusion term of the k equation. (TURB20)
* σ_ϵ	SIGE	Constant used in the diffusion term of the ϵ equation. (TURB20)
τ	TAU(I1,I2)	Current value of the time marching parameter. (TIME1)
$\Delta \tau$	DTAU(I1,I2)	Computational time step size. (TIME1)
* θ'_{max}	THMAX	Maximum θ' coordinate in degrees for polar grid option. (GMTRY1)
* θ'_{min}	THMIN	Minimum θ' coordinate in degrees for polar grid option. (GMTRY1)
* θ_1, θ_2	THC(I)	A two-element array specifying the time difference centering parameters used for the continuity equation. (NUM1)
* θ_1, θ_2	THKE(I)	A two-element array specifying the time difference centering parameters used for the k - ϵ equations. (NUM2)
* $\theta_1, \theta_2, \theta_3$	THE(I)	A three-element array specifying the time difference centering parameters used for the energy equation. (NUM1)
* $\theta_1, \theta_2, \theta_3$	THX(I)	A three-element array specifying the time difference centering parameters used for the x -momentum equation. (NUM1)
* $\theta_1, \theta_2, \theta_3$	THY(I)	A three-element array specifying the time difference centering parameters used for the y or r -momentum equation. (NUM1)
* $\theta_1, \theta_2, \theta_3$	THZ(I)	A three-element array specifying the time difference centering parameters used for the swirl momentum equation. (NUM1)
$ \bar{\Omega} $	VORT(I1,I2)	Total vorticity magnitude. (TURB1)
$ \bar{\Omega} $	VORT(I1,I2)	Production rate of turbulent kinetic energy. (TURB1)

4.0 PROTEUS SUBPROGRAMS

In this section, each subprogram in *Proteus* is described, first in summary, then in detail. The summary is simply a list of the subprograms with a brief description of the purpose of each one. The detailed description includes, for each subprogram, a list of the subprograms that reference it, and a list of the subprograms that it references. The Fortran variables that are input to and output from each subprogram are defined. And finally, details of the computations being done within each subprogram are presented.

4.1 SUBPROGRAM SUMMARY

The following table presents a brief description of the purpose of each subprogram in the *Proteus* code.

Proteus Subprogram Summary	
Subprogram	Purpose
ADI	Manage the block tridiagonal inversion.
AVISC1	Compute constant coefficient artificial viscosity.
AVISC2	Compute nonlinear coefficient artificial viscosity.
BCDENS	Compute density boundary conditions.
BCELIM	Eliminate off-diagonal coefficient submatrices resulting from three-point boundary conditions.
BCF	Compute user-written boundary conditions.
BCFLIN	User-supplied routine for linearization of user-supplied boundary conditions.
BCGEN	Manage computation of boundary conditions.
BCGRAD	Compute gradients with respect to ξ and η .
BCMET	Compute various metric functions for normal gradient boundary conditions.
BCPRES	Compute pressure boundary conditions.
BCQ	Compute conservation variable boundary conditions.
BCSET	Set various boundary condition parameters and flags.
BCTEMP	Compute temperature boundary conditions.
BCUVEL	Compute x-velocity boundary conditions.
BCVDIR	Compute normal and tangential velocity boundary conditions.
BCVVEL	Compute y or r-velocity boundary conditions.
BCWVEL	Compute swirl velocity boundary conditions.
BLIN1	Compute inner layer turbulent viscosity along constant ξ lines.
BLIN2	Compute inner layer turbulent viscosity along constant η lines.
BLKOUT	Print coefficient blocks at specified indices in the ξ and η directions.
BLK2	Solve 2×2 block tridiagonal system of equations.
BLK2P	Solve 2×2 periodic block tridiagonal system of equations.
BLK3	Solve 3×3 block tridiagonal system of equations.
BLK3P	Solve 3×3 periodic block tridiagonal system of equations.

Proteus Subprogram Summary	
Subprogram	Purpose
BLK4	Solve 4×4 block tridiagonal system of equations.
BLK4P	Solve 4×4 periodic block tridiagonal system of equations.
BLK5	Solve 5×5 block tridiagonal system of equations.
BLK5P	Solve 5×5 periodic block tridiagonal system of equations.
BLOCK DATA	Set default values for input parameters, plus a few other parameters.
BLOUT1	Compute outer layer turbulent viscosity along constant ξ lines.
BLOUT2	Compute outer layer turbulent viscosity along constant η lines.
BVUP	Update first sweep boundary values after second sweep.
COEFC	Compute coefficients and source terms for the continuity equation.
COEFE	Compute coefficients and source terms for the energy equation.
COEFS1	Compute coefficients and source terms for the k and ϵ equations for the first ADI sweep.
COEFS2	Compute coefficients and source terms for the k and ϵ equations for the second ADI sweep.
COEFX	Compute coefficients and source terms for the x -momentum equation.
COEFY	Compute coefficients and source terms for the y or r -momentum equation.
COEFZ	Compute coefficients and source terms for the swirl momentum equation.
CONV	Test computed flow field for convergence.
CUBIC	Interpolation using Ferguson's parametric cubic.
EQSTAT	Use equation of state to compute pressure, temperature, and their derivatives with respect to the dependent variables.
EXEC	Manage solution of the mean flow equations.
EXECT	Manage solution of the k - ϵ equations.
FILTER	Rearrange rows of the boundary condition coefficient submatrices and the source term subvector to eliminate any zeroes on the diagonal.
FTEMP	Compute auxiliary variables that are functions of temperature.
GEOM	Manage computation of grid and metric parameters.
INIT	Get user-defined initial flow field.
INITC	Set up consistent initial conditions based on data from INIT.
INPUT	Read and print input, perform various initializations.
ISAMAX	Find the first index corresponding to the largest absolute value of the elements of an vector. This is a Cray search routine.
ISAMIN	Find the first index corresponding to the smallest absolute value of the elements of an vector. This is a Cray search routine.
ISRCHEQ	Find the first index in an array whose element is equal to a specified value. This is a Cray search routine.
KEINIT	Get user-defined initial conditions for k and ϵ .
MAIN	Manage overall solution.
METS	Compute metrics of nonorthogonal grid transformation.

Proteus Subprogram Summary	
Subprogram	Purpose
OUTPUT	Manage printing of output.
OUTW	Compute and print parameters at boundaries.
PAK	Manage packing and/or interpolation of grid points.
PERIOD	Define extra line of data for use in computing coefficients for spatially periodic boundary conditions.
PLOT	Write files for post-processing by CONTOUR or PLOT3D plotting programs.
PRODC	Compute production term for the $k-\epsilon$ turbulence model.
PRTHST	Print convergence history.
PRTOUT	Print output.
RESID	Compute residuals and write convergence history file.
REST	Read and/or write restart file.
ROBTS	Pack points along a line using Roberts transformation.
SASUM	Compute the sum of the absolute values of the elements of a vector. This is a Cray BLAS routine.
SGEFA	Factor a matrix using Gaussian elimination. This is a Cray LINPACK routine.
SGESL	Solve the matrix equation $Ax = B$ or $A^T x = B$ using the factors computed by SGEFA. This is a Cray LINPACK routine.
SNRM2	Compute the L_2 norm of a vector. This is a Cray BLAS routine.
TBC	Set time-dependent boundary condition values.
TIMSTP	Set computational time step.
TREMAIN	Get CPU time remaining for the job. This is a Cray Fortran routine.
TURBBL	Manage computation of turbulence parameters using the Baldwin-Lomax algebraic model.
TURBCH	Manage computation of turbulence parameters using the Chien $k-\epsilon$ model.
UPDATE	Update flow variables after each ADI sweep.
UPDTKE	Update k and ϵ after each time step.
VORTEX	Compute magnitude of total vorticity.
YPLUSN	Compute the distance to the nearest solid wall.

4.2 SUBPROGRAM DETAILS

The subprograms used in *Proteus* are described in detail in the remainder of this section. A few additional words are necessary about the input and output descriptions. The description of the input to each subprogram includes all Fortran variables actually used by the subprogram that are defined outside the subprogram. Variables defined and used inside the subprogram are not listed as input. In addition, common block variables that are merely passed through to lower level routines are not listed. Variables marked with an asterisk are user-specified namelist input variables.

Similarly, the output description includes only those variables computed inside the subprogram and used outside the subprogram. It does not include common block variables computed by lower level routines. In general, variables defined inside the subprogram that are used by lower level routines are listed as output, even if they are not needed after control is returned to the calling program.

Variables entering or leaving a subprogram through an argument list are defined in detail. However, most of the Fortran variables listed in the input and output descriptions are contained in common blocks, and are defined in detail in Section 3.0. For that reason, they are defined only briefly in this section.

Subroutine ADI (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	BLKOUT BLK3 BLK3P BLK4 BLK4P BLK5 BLK5P	Manage the block tridiagonal inversion.

Input

A, B, C	Coefficient submatrices A, B, and C.
* IDEBUG	Debug flags.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ISWEEP	Current ADI sweep number.
IT	Current time step number n .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
NEQ	Number of coupled equations being solved, N_{eq} .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S, and computed solution subvector, $\Delta\hat{Q}$ or $\Delta\hat{Q}^n$.

Output

None.

Description

For each ADI sweep, subroutine ADI calls the appropriate block solver. The choice is determined by the number of equations being solved, and by the presence or absence of spatially periodic boundary conditions in the sweep direction.

Remarks

1. This subroutine generates the output for the IDEBUG(1), IDEBUG(5), and IDEBUG(6) options.

Subroutine AVISC1 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	BLKOUT	Compute constant coefficient artificial viscosity.

Input

A, B, C	Coefficient submatrices A, B, and C without artificial viscosity.
* CAVS2E, CAVS4E, CAVS2I	Artificial viscosity coefficients $\varepsilon_E^{(2)}$, $\varepsilon_E^{(4)}$, and ε_I .
DTAU	Time step $\Delta\tau$.
* IAV2E, IAV4E, IAV2I	Flags for second-order explicit, fourth-order explicit, and second-order implicit artificial viscosity.
* IDEBUG	Debug flags.
* IHSTAG	Flag for constant stagnation enthalpy option.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IT	Current time step number n .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
NC, NXM, NYM, NZM, NEN	Array indices associated with the continuity, x -momentum, y -momentum (or r -momentum if axisymmetric), swirl momentum, and energy equations.
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
S	Source term subvector S without artificial viscosity.

Output

A, B, C	Coefficient submatrices A, B, and C with artificial viscosity.
S	Source term subvector S with artificial viscosity.

Description

Subroutine AVISC1 adds explicit and/or implicit artificial viscosity to the governing equations, using the constant coefficient model of Steger (1978), as presented by Pulliam (1986b). The model is described in Section 8.1 of Volume 1. The explicit artificial viscosity may be second and/or fourth order, and is added only during the first ADI sweep. The implicit artificial viscosity is second order, and is added during both sweeps.

The fourth-order explicit artificial viscosity is implemented in Fortran by redefining the source term subvector as

$$S_{i,j} = S_{i,j} - \frac{\varepsilon_E^{(4)} \Delta \tau_{i,j}}{J_{i,j}} [(\nabla_\xi \Delta_\xi)^2 Q_{i,j} + (\nabla_\eta \Delta_\eta)^2 Q_{i,j}]$$

where i and j vary from 3 to NPT1 - 2 and from 3 to NPT2 - 2, respectively. At grid points adjacent to boundaries the fourth-order differences in the above equation cannot be used, and therefore are replaced by second-order differences. Thus, at $i = 2$ and at $i = \text{NPT1} - 1$, with j varying from 3 to NPT2 - 2,

$$S_{i,j} = S_{i,j} + \frac{\varepsilon_E^{(4)} \Delta \tau_{i,j}}{J_{i,j}} [\nabla_\xi \Delta_\xi Q_{i,j} - (\nabla_\eta \Delta_\eta)^2 Q_{i,j}]$$

Similarly, at $j = 2$ and at $j = \text{NPT2} - 1$, with i varying from 3 to NPT1 - 1,

$$S_{i,j} = S_{i,j} + \frac{\varepsilon_E^{(4)} \Delta \tau_{i,j}}{J_{i,j}} [- (\nabla_\xi \Delta_\xi)^2 Q_{i,j} + \nabla_\eta \Delta_\eta Q_{i,j}]$$

The second-order explicit artificial viscosity is implemented in Fortran by redefining the source term subvector as

$$S_{i,j} = S_{i,j} + \frac{\varepsilon_E^{(2)} \Delta \tau_{i,j}}{J_{i,j}} (\nabla_\xi \Delta_\xi Q_{i,j} + \nabla_\eta \Delta_\eta Q_{i,j})$$

where i and j vary from 2 to NPT1 - 1 and from 2 to NPT2 - 1, respectively.

The second-order implicit artificial viscosity for the first ADI sweep is implemented in Fortran by redefining the coefficient block submatrices as

$$\begin{aligned} A_{i,j} &= A_{i,j} - \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i-1,j} \\ B_{i,j} &= B_{i,j} + 2 \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i,j} \\ C_{i,j} &= C_{i,j} - \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i+1,j} \end{aligned}$$

where i and j vary from 2 to NPT1 - 1 and from 2 to NPT2 - 1, respectively. Similarly, for the second sweep,

$$\begin{aligned} A_{i,j} &= A_{i,j} - \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i,j-1} \\ B_{i,j} &= B_{i,j} + 2 \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i,j} \\ C_{i,j} &= C_{i,j} - \frac{\varepsilon_I \Delta \tau_{i,j}}{J_{i,j}} J_{i,j+1} \end{aligned}$$

Remarks

1. The sign in front of each artificial viscosity term depends on the sign of the " i,j " term in the difference formula. See Section 8.1 of Volume 1 for details.

2. The coding to add artificial viscosity to the energy and/or swirl momentum equations is separate from the coding for the remaining equations, and is bypassed if they are not being solved.
3. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For the first sweep (which includes all the explicit artificial viscosity) the order is thus (I2,I1), and for the second sweep the order is (I1,I2).
4. For spatially periodic boundary conditions in the ξ direction, fourth-order differences could be used at $i = 2$ and at $i = \text{NPT1} - 1 (= N_1)$. Similarly, for the η direction, fourth-order differences could be used at $j = 2$ and at $j = \text{NPT2} - 1 (= N_2)$. The logic to do this has not been coded, however, and at these points second-order differences are still used, as described above.
5. This subroutine generates the output for the IDEBUG(2) option.

Subroutine AVISC2 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	BLKOUT	Compute nonlinear coefficient artificial viscosity.

Input

A, B, C	Coefficient submatrices A , B , and C .
* CAVS2E, CAVS4E	User-specified coefficients κ_2 and κ_4 .
CP, CV	Specific heats c_p and c_v at time level n .
DTAU	Time step $\Delta\tau$.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* IAV2E, IAV4E	Flags for second-order and fourth-order explicit artificial viscosity.
* IDEBUG	Debug flags.
* IHSTAG	Flag for constant stagnation enthalpy option.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IT	Current time step number n .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
NC, NXM, NYM, NZM, NEN	Array indices associated with the continuity, x -momentum, y -momentum (or r -momentum if axisymmetric), swirl momentum, and energy equations.
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
NVD, NPTSD	Leading two dimensions for the arrays A , B , C , and S .
P, T	Static pressure p and temperature T at time level n .
RGAS	Gas constant R .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
S	Source term subvector S without artificial viscosity.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .

Output

S	Source term subvector S with artificial viscosity.
---	---

Description

Subroutine AVISC2 adds explicit artificial viscosity to the governing equations, using the nonlinear coefficient model of Jameson, Schmidt, and Turkel (1981), as presented by Pulliam (1986b). The model is described in Section 8.2 of Volume 1. Implicit artificial viscosity is not normally used in combination with

the explicit nonlinear coefficient model. The explicit artificial viscosity is added only during the first ADI sweep.

The artificial viscosity in the ξ direction is computed first, at the η -indices $j = 2$ to $\text{NPT2} - 1$. The spectral radius term $\psi_{i,j}$ and the pressure gradient scaling factor $\sigma_{i,j}$ are computed and stored in local one-dimensional arrays for $i = 1$ to NPT1 . Special formulas are used to compute σ near boundaries, as described in Section 8.2 of Volume 1.

The second-order artificial viscosity is added first, and is implemented in Fortran by redefining the source term subvector as

$$S_{i,j} = S_{i,j} + \nabla_{\xi} \left\{ \left[\left(\frac{\psi}{J} \right)_{i+1,j} + \left(\frac{\psi}{J} \right)_{i,j} \right] (\varepsilon_{\xi}^{(2)})_{i,j} \Delta_{\xi} Q_{i,j} \right\}$$

Or, after evaluating the differences,

$$S_{i,j} = S_{i,j} + \left[\left(\frac{\psi}{J} \right)_{i+1,j} + \left(\frac{\psi}{J} \right)_{i,j} \right] (\varepsilon_{\xi}^{(2)})_{i,j} (Q_{i+1,j} - Q_{i,j}) \\ - \left[\left(\frac{\psi}{J} \right)_{i,j} + \left(\frac{\psi}{J} \right)_{i-1,j} \right] (\varepsilon_{\xi}^{(2)})_{i-1,j} (Q_{i,j} - Q_{i-1,j})$$

where i varies from 2 to $\text{NPT1} - 1$.

The fourth-order artificial viscosity is added next, and is implemented similarly by redefining the source term subvector as

$$S_{i,j} = S_{i,j} - \nabla_{\xi} \left\{ \left[\left(\frac{\psi}{J} \right)_{i+1,j} + \left(\frac{\psi}{J} \right)_{i,j} \right] (\varepsilon_{\xi}^{(4)})_{i,j} \Delta_{\xi} \nabla_{\xi} \Delta_{\xi} Q_{i,j} \right\}$$

Or, after evaluating the differences,

$$S_{i,j} = S_{i,j} - \left[\left(\frac{\psi}{J} \right)_{i+1,j} + \left(\frac{\psi}{J} \right)_{i,j} \right] (\varepsilon_{\xi}^{(4)})_{i,j} (Q_{i+2,j} - 3Q_{i+1,j} + 3Q_{i,j} - Q_{i-1,j}) \\ + \left[\left(\frac{\psi}{J} \right)_{i,j} + \left(\frac{\psi}{J} \right)_{i-1,j} \right] (\varepsilon_{\xi}^{(4)})_{i-1,j} (Q_{i+1,j} - 3Q_{i,j} + 3Q_{i-1,j} - Q_{i-2,j})$$

where i varies from 3 to $\text{NPT1} - 2$. Special formulas are used at $i = 2$ and at $i = \text{NPT1} - 1$, as described in Section 8.2 of Volume 1.

The artificial viscosity in the η direction is computed next, and is implemented in a manner analogous to that just described for the artificial viscosity in the ξ direction.

Remarks

1. The sign in front of each artificial viscosity term depends on the sign of the " i,j " term in the difference formula. See Section 8.1 of Volume 1 for details.
2. The coding to add artificial viscosity to the energy and/or swirl momentum equations is separate from the coding for the remaining equations, and is bypassed if they are not being solved.
3. The subscripts on the Fortran variable S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For the first sweep (which includes all the explicit artificial viscosity) the order is thus (I2,I1).

4. For spatially periodic boundary conditions, the need for special formulas near boundaries could be eliminated. The logic to do this has not been coded, however.
5. This subroutine generates the output for the IDEBUG(2) option.

Subroutine BCDENS (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute density boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i_v .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR	Array index associated with the dependent variable ρ .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
RHO	Static density ρ at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCDENS computes coefficients and source terms for density boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular density boundary conditions in *Proteus*.⁷

⁷ In the following description, for the first ADI sweep the dependent variable should have the superscript *, representing the intermediate solution, and for the second ADI sweep it should have the superscript n , representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

No Change From Initial Conditions, $\Delta\rho = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g/\partial \hat{Q} = J\partial g/\partial Q$, we get simply

$$J_{i,j} \Delta \hat{\rho}_{i,j}^n = 0$$

Specified Static Density, $\rho = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \Delta \hat{\rho}_{i,j}^n = f_{i,j}^{n+1} - \rho_{i,j}^n$$

Specified Two-Point Density Gradient in Coordinate Direction, $\partial\rho/\partial\phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$-J_{1,j} \Delta \hat{\rho}_{1,j}^n + J_{2,j} \Delta \hat{\rho}_{2,j}^n = (\Delta\xi) f_{1,j}^{n+1} + \rho_{1,j}^n - \rho_{2,j}^n$$

At the $\xi = 1$ boundary,

$$-J_{N_1-1,j} \Delta \hat{\rho}_{N_1-1,j}^n + J_{N_1,j} \Delta \hat{\rho}_{N_1,j}^n = (\Delta\xi) f_{N_1,j}^{n+1} + \rho_{N_1-1,j}^n - \rho_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Density Gradient in Coordinate Direction, $\partial\rho/\partial\phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$-3J_{1,j} \Delta \hat{\rho}_{1,j}^n + 4J_{2,j} \Delta \hat{\rho}_{2,j}^n - J_{3,j} \Delta \hat{\rho}_{3,j}^n = 2(\Delta\xi) f_{1,j}^{n+1} + 3\rho_{1,j}^n - 4\rho_{2,j}^n + \rho_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \Delta \hat{\rho}_{N_1-2,j}^n - 4J_{N_1-1,j} \Delta \hat{\rho}_{N_1-1,j}^n + 3J_{N_1,j} \Delta \hat{\rho}_{N_1,j}^n = 2(\Delta\xi) f_{N_1,j}^{n+1} - \rho_{N_1-2,j}^n + 4\rho_{N_1-1,j}^n - 3\rho_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Density Gradient in Normal Direction, $\nabla\rho \cdot \bar{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$-J_{1,j} \Delta \hat{\rho}_{1,j}^n + J_{2,j} \Delta \hat{\rho}_{2,j}^n = \frac{\Delta\xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta \rho_{1,j}^n \right] + \rho_{1,j}^n - \rho_{2,j}^n$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$-J_{N_1-1,j} \Delta \hat{\rho}_{N_1-1,j}^n + J_{N_1,j} \Delta \hat{\rho}_{N_1,j}^n = \frac{\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta \rho_{N_1,j}^n \right] + \rho_{N_1-1,j}^n - \rho_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Density Gradient in Normal Direction, $\nabla \rho \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$-3J_{1,j}\Delta\hat{\rho}_{1,j}^n + 4J_{2,j}\Delta\hat{\rho}_{2,j}^n - J_{3,j}\Delta\hat{\rho}_{3,j}^n = \frac{2\Delta\xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{1,j}}{m_{1,j}} \delta_\eta \rho_{1,j}^n \right] + 3\rho_{1,j}^n - 4\rho_{2,j}^n + \rho_{3,j}^n$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$J_{N_1-2,j}\Delta\hat{\rho}_{N_1-2,j}^n - 4J_{N_1-1,j}\Delta\hat{\rho}_{N_1-1,j}^n + 3J_{N_1,j}\Delta\hat{\rho}_{N_1,j}^n = \frac{2\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta \rho_{N_1,j}^n \right] - \rho_{N_1-2,j}^n + 4\rho_{N_1-1,j}^n - 3\rho_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Static Density

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$J_{1,j}\Delta\hat{\rho}_{1,j}^n - 2J_{2,j}\Delta\hat{\rho}_{2,j}^n + J_{3,j}\Delta\hat{\rho}_{3,j}^n = -\rho_{1,j}^n + 2\rho_{2,j}^n - \rho_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j}\Delta\hat{\rho}_{N_1-2,j}^n - 2J_{N_1-1,j}\Delta\hat{\rho}_{N_1-1,j}^n + J_{N_1,j}\Delta\hat{\rho}_{N_1,j}^n = -\rho_{N_1-2,j}^n + 2\rho_{N_1-1,j}^n - \rho_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent density boundary condition is specified.

Subroutine BCELIM (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	SGEFA SGESL	Eliminate off-diagonal coefficient submatrices resulting from three-point boundary conditions.

Input

A, B, C	Coefficient submatrices A, B, and C before eliminating off-diagonal blocks.
IBCELM	Flags for elimination of off-diagonal coefficient submatrices resulting from three-point boundary conditions in the ξ and η directions at either boundary; 0 if elimination is not necessary, 1 if it is.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i .
NEQ	Number of coupled equations being solved, N_{eq} .
NEQP	Dimensioning parameter specifying maximum number of coupled equations allowed.
NPTS	Number of grid points in the sweep direction, N .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S before eliminating off-diagonal blocks.

Output

A, B, C	Coefficient submatrices A, B, and C after eliminating off-diagonal blocks.
S	Source term subvector S after eliminating off-diagonal blocks.

Description

Subroutine BCELIM eliminates the off-diagonal coefficient submatrices that result from the application of three-point boundary conditions. This is necessary when three-point gradients are specified in the coordinate or normal direction, and when linear extrapolation is used. The procedure is described in Section 7.2.1 of Volume 1.

Remarks

1. Subroutines SGEFA and SGESL are Cray LINPACK routines. In general terms, if the Fortran arrays A and B represent \mathbf{A} and \mathbf{B} , where \mathbf{A} is a square N by N matrix and \mathbf{B} is a matrix (or vector) with $NCOL$ columns, and if the leading dimension of the Fortran array A is LDA , then the Fortran sequence

```

10      call sgefa (a,lda,n,ipvt,info)
        do 10 j = 1,ncol
          call sgesl (a,lda,n,ipvt,b(1,j),0)
        continue
```

computes $\mathbf{A}^{-1}\mathbf{B}$, storing the result in \mathbf{B} .

Subroutine BCF (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCFLIN BCMET	Compute user-written boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
* IHSTAG	Flag for constant stagnation enthalpy option.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NK, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCF computes coefficients and source terms for user-written boundary conditions of the form $\Delta F = 0$, $F = f$, $\partial F / \partial \phi = f$, and $\nabla F \cdot \vec{n} = f$. The values of F and its derivatives with respect to the dependent variables must be supplied by the user-written subroutine BCFLIN. The linearized equations for these types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections expand these generalized equations in detail.⁸

⁸ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n , representing

No Change From Initial Conditions, $\Delta F = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{Q} = J \partial g / \partial Q$, we get simply

$$J_{i,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = 0$$

Specified Value, $F = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = f_{i,j}^{n+1} - F_{i,j}^n$$

Specified Two-Point Gradient in Coordinate Direction, $\partial F / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -J_{1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\ & J_{2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\ & (\Delta \xi) f_{1,j}^{n+1} + F_{1,j}^n - F_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} & -J_{N_1-1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\ & J_{N_1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\ & (\Delta \xi) f_{N_1,j}^{n+1} + F_{N_1-1,j}^n - F_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Gradient in Coordinate Direction, $\partial F / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& 2(\Delta \xi) f_{1,j}^{n+1} + 3F_{1,j}^n - 4F_{2,j}^n + F_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& 2(\Delta \xi) f_{N_1,j}^{n+1} - F_{N_1-2,j}^n + 4F_{N_1-1,j}^n - 3F_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Gradient in Normal Direction, $\nabla F \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned}
& -J_{1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& J_{2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\
& \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta F_{1,j}^n \right] + F_{1,j}^n - F_{2,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& -J_{N_1-1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& J_{N_1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta F_{N_1,j}^n \right] + F_{N_1-1,j}^n - F_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Gradient in Normal Direction, $\nabla F \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta F_{1,j}^n \right] + 3F_{1,j}^n - 4F_{2,j}^n + F_{3,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{2\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta F_{N_1,j}^n \right] - F_{N_1-2,j}^n + 4F_{N_1-1,j}^n - 3F_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$\begin{aligned}
 & J_{1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n - \\
 & 2J_{2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n + \\
 & J_{3,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
 & -F_{1,j}^n + 2F_{2,j}^n - F_{3,j}^n
 \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
 & J_{N_1-2,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
 & 2J_{N_1-1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
 & J_{N_1,j} \left[\frac{\partial F}{\partial \rho} \Delta \hat{\rho} + \frac{\partial F}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial F}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial F}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial F}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
 & -F_{N_1-2,j}^n + 2F_{N_1-1,j}^n - F_{N_1,j}^n
 \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent user-written boundary condition is specified.

Subroutine BCFLIN (IBC,IEQ,IBOUND,IMIN,IMAX,F,DFDRHO,DFDRU,DFDRV,DFDRW,DFDET,FBCM,FBCP,FBC)		
Called by	Calls	Purpose
BCF		User-supplied routine for linearization of user-supplied boundary conditions.

Input

IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC	Mean flow boundary condition types for current sweep direction, specified as IBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
I1, I2	Grid indices i and j , in the ξ and η directions.
N1P	Parameter specifying the dimension size in the ξ direction.

Output

DFDRHO, DFDRU, DFDRV, DFDRW, DFDET	Three-element arrays, specified as DFDRHO(IW), etc., giving the values of $\partial F/\partial \rho$, $\partial F/\partial(\rho u)$, $\partial F/\partial(\rho v)$, $\partial F/\partial(\rho w)$, and $\partial F/\partial E_T$.
F	A three-element array specified as F(IW) giving the value of the function F at the boundary (IW = 1), at the first point away from the boundary (IW = 2), and at the second point away from the boundary (IW = 3). Values at IW = 3 are not needed for boundary condition types 91, 92, or -92. Values at IW = 2 are not needed for boundary condition type 91.
FBC	Boundary condition values for current sweep direction, specified as FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries. This is only needed if values for GBC1 or GBC2, or FBC1 or FBC2, are not specified in the input namelist BC.
FBCM, FBCP	Boundary condition values on the boundary, at the grid points "below" and "above" the current boundary point. These are only needed for boundary condition types ± 93 .

Description

Subroutine BCFLIN is a user-written routine used in conjunction with subroutine BCF for user-written boundary conditions of the form $\Delta F = 0$, $F = f$, $\partial F/\partial \phi = f$, and $\nabla F \cdot \vec{n} = f$. BCFLIN supplies the values of F and its derivatives with respect to the dependent variables, which are required for writing the linearized form of the boundary condition.

The version of BCFLIN supplied with *Proteus* makes BCF equivalent to BCTEMP, except for the total temperature options in BCTEMP. Thus $F = T$, $\partial F / \partial \rho = \partial T / \partial \rho$, etc., where T and its derivatives with respect to the dependent variables are computed using the perfect gas equation of state. (See Section 4.3 of Volume 1.) This version of BCFLIN is intended as an example for use in coding boundary conditions not already available.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The capability of specifying FBC as an output variable may be useful in writing time-dependent boundary conditions. It also may be used when specifying boundary conditions involving derivatives in both coordinate directions. In this case, the derivatives in the non-sweep direction may be lagged one time step and treated as source terms.

Subroutine BCGEN (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
BVUP EXEC	BCDENS BCF BCPRES BCQ BCTEMP BCUVEL BCVDIR BCVVEL BCWVEL BLKOUT ISRCHEQ	Manage computation of boundary conditions.

Input

A, B, C	Coefficient submatrices A, B, and C.
* FBC1, FBC2	Point-by-point mean flow boundary condition values for the ξ and η directions.
* IBC1, IBC2	Point-by-point mean flow boundary condition types for the ξ and η directions.
* IDEBUG	Debug flags.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ISWEEP	Current ADI sweep number.
IT	Current time step number n .
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
NBC	Dimensioning parameter specifying number of boundary conditions per equation.
NEQ	Number of coupled equations being solved, N_{eq} .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
S	Source term subvector S.

Output

IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.

IEQ

Boundary condition equation number, from 1 to N_{eq} .

IMIN, IMAX

Minimum and maximum indices in the sweep direction.

Description

Subroutine BCGEN manages the computation of coefficients and source terms for the mean flow boundary conditions. It first loads the NEQ boundary condition types and values from the input arrays IBC1 and FBC1, or IBC2 and FBC2, depending on the ADI sweep, into the arrays IBC and FBC. This was done so that the BC routines could be non-sweep dependent. Next the coefficient submatrices and source term subvectors at the two boundaries in the current sweep direction are initialized to zero. And finally, the appropriate BC routine is called, depending on the input boundary condition type, for each of the NEQ boundary conditions at each boundary in the sweep direction.

Remarks

1. An error message is generated and execution is stopped if any of the non-existent boundary condition types 80-89 is specified, or if the boundary condition type is less than 0 or greater than 99.
2. The Cray search routine ISRCHEQ is used in determining the grid locations for debug printout.
3. This subroutine generates the output for the IDEBUG(3) option.

Subroutine BCGRAD (F,I,DFD1,DFD2)		
Called by	Calls	Purpose
BCDENS BCF BCPRES BCQ BCTEMP BCUVEL BCVDIR BCVVEL BCWVEL		Compute gradients with respect to ξ and η .

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
F	A two-dimensional array, specified as F(I,J), containing the function f whose gradient is to be computed. The subscripts I and J run from 1 to N_1 and N_2 , respectively.
I	Current grid point index in the current sweep direction.
ISWEEP	Current ADI sweep number.
I1, I2	Grid indices i and j , in the ξ and η directions.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.

Output

DFD1, DFD2	First derivatives of f with respect to ξ and η .
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Description

Subroutine BCGRAD computes first derivatives of the function f , with respect to ξ and η , at the current grid point in the ADI sweep direction. At interior points, the centered difference formula presented in Section 5.0 of Volume 1 is used. For derivatives with respect to ξ ,

$$\left(\frac{\partial f}{\partial \xi} \right)_{i,j} \simeq \frac{f_{i+1,j} - f_{i-1,j}}{\Delta \xi}$$

An analogous formula is used for η derivatives.

At boundary points three-point one-sided formulas are used.

$$\left(\frac{\partial f}{\partial \xi} \right)_{1,j} \simeq \frac{1}{2\Delta \xi} (-3f_{1,j} + 4f_{2,j} - f_{3,j})$$

$$\left(\frac{\partial f}{\partial \xi} \right)_{N_1,j} \simeq \frac{1}{2\Delta \xi} (f_{N_1-2,j} - 4f_{N_1-1,j} + 3f_{N_1,j})$$

Again, analogous formulas are used for η derivatives.

Subroutine BCMET (I,FM0,FM1,FM2)		
Called by	Calls	Purpose
BCDENS BCF BCPRES BCQ BCTEMP BCUVEL BCVDIR BCVVEL BCWVEL		Compute various metric functions for normal gradient boundary conditions.

Input

ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric.)
I	Current grid point index in the current sweep direction.
ISWEEP	Current ADI sweep number.
I1, I2	Grid indices i and j , in the ξ and η directions.
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ_r if axisymmetric.)

Output

FM0, FM1, FM2	Various metric functions used for normal derivative boundary conditions.
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Description

Subroutine BCMET computes metric functions used for normal gradient boundary conditions. For the first ADI sweep,

$$\begin{aligned} FM0 &= \sqrt{\xi_x^2 + \xi_y^2} \\ FM1 &= 0 \\ FM2 &= \xi_x \eta_x + \xi_y \eta_y \end{aligned}$$

And for the second sweep,

$$\begin{aligned} FM0 &= \sqrt{\eta_x^2 + \eta_y^2} \\ FM1 &= \xi_x \eta_x + \xi_y \eta_y \\ FM2 &= 0 \end{aligned}$$

Subroutine BCPRES (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute pressure boundary conditions.

Input

CP, CV	Specific heats c_p and c_v at time level n .
DEL	Computational grid spacing in sweep direction.
DPDRHO, DPDRU, DPDRV, DPDRW, DPDET	Derivatives $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, $\partial p/\partial(\rho v)$, $\partial p/\partial(\rho w)$, and $\partial p/\partial E_T$.
DTDRHO, DTDRU, DTDRV, DTDRW, DTDET	Derivatives $\partial T/\partial \rho$, $\partial T/\partial(\rho u)$, $\partial T/\partial(\rho v)$, $\partial T/\partial(\rho w)$, and $\partial T/\partial E_T$.
GC	Proportionality factor g_c in Newton's second law.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
* IHSTAG	Flag for constant stagnation enthalpy option.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i_v .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
P, T	Static pressure p and temperature T at time level n .
PR	Reference pressure p_r .
RGAS	Gas constant R .
RHO, U, V, W	Static density ρ , and velocities u , v , and w , at time level n .
* RHOR, UR	Reference density ρ_r and velocity u_r .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
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S

Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCPRES computes coefficients and source terms for pressure boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular pressure boundary conditions in *Proteus*.⁹

No Change From Initial Conditions, $\Delta p = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{\mathbf{Q}} = J \partial g / \partial \mathbf{Q}$, we get simply

$$J_{i,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = 0$$

The derivatives $\partial p / \partial \rho$, $\partial p / \partial (\rho u)$, etc., depend on the equation of state. They are defined for a perfect gas in Section 4.3 of Volume 1.

Specified Static Pressure, $p = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = f_{i,j}^{n+1} \frac{p_r g_c}{\rho_r \mu_r^2} - p_{i,j}^n$$

Specified Two-Point Pressure Gradient in Coordinate Direction, $\partial p / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -J_{1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\ & J_{2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\ & (\Delta \xi) f_{1,j}^{n+1} \frac{p_r g_c}{\rho_r \mu_r^2} + p_{1,j}^n - p_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

⁹ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n, representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

$$\begin{aligned}
& -J_{N_1-1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& J_{N_1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& (\Delta \xi) f_{N_1,j}^{n+1} \frac{Pr g_c}{\rho_r \mu_r^2} + p_{N_1-1,j}^n - p_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Pressure Gradient in Coordinate Direction, $\partial p / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& 2(\Delta \xi) f_{1,j}^{n+1} \frac{Pr g_c}{\rho_r \mu_r^2} + 3p_{1,j}^n - 4p_{2,j}^n + p_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& 2(\Delta \xi) f_{N_1,j}^{n+1} \frac{Pr g_c}{\rho_r \mu_r^2} - p_{N_1-2,j}^n + 4p_{N_1-1,j}^n - 3p_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Pressure Gradient in Normal Direction, $\nabla p \cdot \tilde{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned}
& -J_{1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& J_{2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\
& \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} \frac{p_r g_c}{\rho_r u_r^2} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta p_{1,j}^n \right] + p_{1,j}^n - p_{2,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& -J_{N_1-1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& J_{N_1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} \frac{p_r g_c}{\rho_r u_r^2} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta p_{N_1,j}^n \right] + p_{N_1-1,j}^n - p_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Pressure Gradient in Normal Direction, $\nabla p \cdot \bar{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} \frac{p_r g_c}{\rho_r u_r^2} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta p_{1,j}^n \right] + 3p_{1,j}^n - 4p_{2,j}^n + p_{3,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{2\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} \frac{p_T g_c}{\rho_T u_T^2} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta p_{N_1,j}^n \right] - p_{N_1-2,j}^n + 4p_{N_1-1,j}^n - 3p_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Static Pressure

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$\begin{aligned}
& J_{1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n - \\
& 2J_{2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n + \\
& J_{3,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& -p_{1,j}^n + 2p_{2,j}^n - p_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 2J_{N_1-1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& J_{N_1,j} \left[\frac{\partial p}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& -p_{N_1-2,j}^n + 2p_{N_1-1,j}^n - p_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

No Change From Initial Conditions for Total Pressure, $\Delta p_T = 0$

The total pressure is defined as

$$p_T = p \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}}$$

Applying equation (6.3) of Volume 1, we get

$$J_{i,j} \left[\frac{\partial p_T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p_T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p_T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p_T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p_T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = 0$$

where

$$\begin{aligned} \frac{\partial p_T}{\partial \rho} &= \frac{\partial p}{\partial \rho} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}} + p \frac{\gamma}{2} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1}{\gamma-1}} \frac{\partial M^2}{\partial \rho} \\ \frac{\partial p_T}{\partial(\rho u)} &= \frac{\partial p}{\partial(\rho u)} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}} + p \frac{\gamma}{2} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1}{\gamma-1}} \frac{\partial M^2}{\partial(\rho u)} \\ \frac{\partial p_T}{\partial(\rho v)} &= \frac{\partial p}{\partial(\rho v)} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}} + p \frac{\gamma}{2} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1}{\gamma-1}} \frac{\partial M^2}{\partial(\rho v)} \\ \frac{\partial p_T}{\partial(\rho w)} &= \frac{\partial p}{\partial(\rho w)} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}} + p \frac{\gamma}{2} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1}{\gamma-1}} \frac{\partial M^2}{\partial(\rho w)} \\ \frac{\partial p_T}{\partial E_T} &= \frac{\partial p}{\partial E_T} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{\gamma}{\gamma-1}} + p \frac{\gamma}{2} \left(1 + \frac{\gamma-1}{2} M^2 \right)^{\frac{1}{\gamma-1}} \frac{\partial M^2}{\partial E_T} \end{aligned}$$

The Mach number is defined by

$$M^2 = \frac{u^2 + v^2 + w^2}{\gamma R T} = \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{\gamma R \rho^2 T}$$

The derivatives $\partial M^2 / \partial \rho$, etc., can then be derived as

$$\begin{aligned} \frac{\partial M^2}{\partial \rho} &= -M^2 \left(\frac{2}{\rho} + \frac{1}{T} \frac{\partial T}{\partial \rho} \right) \\ \frac{\partial M^2}{\partial(\rho u)} &= \frac{2u}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho u)} \\ \frac{\partial M^2}{\partial(\rho v)} &= \frac{2v}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho v)} \\ \frac{\partial M^2}{\partial(\rho w)} &= \frac{2w}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho w)} \\ \frac{\partial M^2}{\partial E_T} &= -\frac{M^2}{T} \frac{\partial T}{\partial E_T} \end{aligned}$$

Specified Total Pressure, $p_T = f$

Applying equation (6.5) of Volume 1, we get

$$J_{i,j} \left[\frac{\partial p_T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial p_T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial p_T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial p_T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial p_T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n =$$

$$f_{i,j}^{n+1} \frac{p_r g_c}{\rho_r u_r^2} - p_{i,j}^n \left[\left(1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{\gamma}{\gamma - 1}} \right]_{i,j}^n$$

where p_T , $\partial p_T / \partial \rho$, etc., are defined above as part of the description of the $\Delta p_T = 0$ boundary condition.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent pressure boundary condition is specified.
3. The multiplying factor $p_r g_c / \rho_r u_r^2$ that appears with specified values of pressure and pressure gradients is necessary because input values of pressure are nondimensionalized by the reference pressure $p_r = \rho_r R T_r / g_c$, while internal to the *Proteus* code itself pressure is nondimensionalized by the normalizing pressure $p_n = \rho_r u_r^2$. (See Section 3.1.1 of Volume 2.)

Subroutine BCQ (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCMET	Compute conservation variable boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
J1	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
NC, NXM, NYM, NZM, NEN	Array indices associated with the continuity, x-momentum, y-momentum (or r-momentum if axisymmetric), swirl momentum, and energy equations.
* NOUT	Unit number for standard output.
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
N1P	Parameter specifying the dimension size in the ξ direction.
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCQ computes coefficients and source terms for conservation variable boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0

of Volume 1. The following sections apply these generalized equations to the particular conservation variable boundary conditions in *Proteus*.¹⁰

No Change From Initial Conditions, $\Delta Q = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{Q} = J \partial g / \partial Q$, we get simply

$$J_{i,j} \Delta \hat{Q}_{i,j}^n = 0$$

where \hat{Q} is the element of \hat{Q} for which this boundary condition is to be applied.

Specified Conservation Variable, $Q = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \Delta \hat{Q}_{i,j}^n = f_{i,j}^{n+1} - Q_{i,j}^n$$

Specified Two-Point Conservation Variable Gradient in Coordinate Direction, $\partial Q / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$-J_{1,j} \Delta \hat{Q}_{1,j}^n + J_{2,j} \Delta \hat{Q}_{2,j}^n = (\Delta \xi) f_{1,j}^{n+1} + Q_{1,j}^n - Q_{2,j}^n$$

At the $\xi = 1$ boundary,

$$-J_{N_1-1,j} \Delta \hat{Q}_{N_1-1,j}^n + J_{N_1,j} \Delta \hat{Q}_{N_1,j}^n = (\Delta \xi) f_{N_1,j}^{n+1} + Q_{N_1-1,j}^n - Q_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Conservation Variable Gradient in Coordinate Direction, $\partial Q / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$-3J_{1,j} \Delta \hat{Q}_{1,j}^n + 4J_{2,j} \Delta \hat{Q}_{2,j}^n - J_{3,j} \Delta \hat{Q}_{3,j}^n = 2(\Delta \xi) f_{1,j}^{n+1} + 3Q_{1,j}^n - 4Q_{2,j}^n + Q_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \Delta \hat{Q}_{N_1-2,j}^n - 4J_{N_1-1,j} \Delta \hat{Q}_{N_1-1,j}^n + 3J_{N_1,j} \Delta \hat{Q}_{N_1,j}^n = 2(\Delta \xi) f_{N_1,j}^{n+1} - Q_{N_1-2,j}^n + 4Q_{N_1-1,j}^n - 3Q_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Conservation Variable Gradient in Normal Direction, $\nabla Q \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

¹⁰ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n, representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

$$-J_{1,j}\Delta\hat{Q}_{1,j}^n + J_{2,j}\Delta\hat{Q}_{2,j}^n = \frac{\Delta\xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{1,j}}{m_{1,j}} \delta_\eta Q_{1,j}^n \right] + Q_{1,j}^n - Q_{2,j}^n$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$-J_{N_1-1,j}\Delta\hat{Q}_{N_1-1,j}^n + J_{N_1,j}\Delta\hat{Q}_{N_1,j}^n = \frac{\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta Q_{N_1,j}^n \right] + Q_{N_1-1,j}^n - Q_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Conservation Variable Gradient in Normal Direction, $\nabla Q \cdot \bar{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} & -3J_{1,j}\Delta\hat{Q}_{1,j}^n + 4J_{2,j}\Delta\hat{Q}_{2,j}^n - J_{3,j}\Delta\hat{Q}_{3,j}^n = \\ & \frac{2\Delta\xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{1,j}}{m_{1,j}} \delta_\eta Q_{1,j}^n \right] + 3Q_{1,j}^n - 4Q_{2,j}^n + Q_{3,j}^n \end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} & J_{N_1-2,j}\Delta\hat{Q}_{N_1-2,j}^n - 4J_{N_1-1,j}\Delta\hat{Q}_{N_1-1,j}^n + 3J_{N_1,j}\Delta\hat{Q}_{N_1,j}^n = \\ & \frac{2\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x\eta_x + \xi_y\eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta Q_{N_1,j}^n \right] - Q_{N_1-2,j}^n + 4Q_{N_1-1,j}^n - 3Q_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Conservation Variable

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$J_{1,j}\Delta\hat{Q}_{1,j}^n - 2J_{2,j}\Delta\hat{Q}_{2,j}^n + J_{3,j}\Delta\hat{Q}_{3,j}^n = -Q_{1,j}^n + 2Q_{2,j}^n - Q_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j}\Delta\hat{Q}_{N_1-2,j}^n - 2J_{N_1-1,j}\Delta\hat{Q}_{N_1-1,j}^n + J_{N_1,j}\Delta\hat{Q}_{N_1,j}^n = -Q_{N_1-2,j}^n + 2Q_{N_1-1,j}^n - Q_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent conservation variable boundary condition is specified.

Subroutine BCSET		
Called by	Calls	Purpose
MAIN		Set various boundary condition parameters and flags.

Input

- * GBC1, GBC2 Surface mean flow boundary condition values for the ξ and η directions.
- * GBCT1, GBCT2 Surface k - ε boundary condition values for the ξ and η directions.
- * GTBC1, GTBC2 Time-dependent surface mean flow boundary condition values for the ξ and η directions.
- * IHSTAG Flag for constant stagnation enthalpy option.
- * ISWIRL Flag for swirl in axisymmetric flow.
- ITDBC Flag for time-dependent mean flow boundary conditions; 0 if all boundary conditions are steady, 1 if any general unsteady boundary conditions are used, 2 if only steady and time-periodic boundary conditions are used.
- * ITURB Flag for turbulent flow option.
- * JBC1, JBC2 Surface mean flow boundary condition types for the ξ and η directions.
- * JBCT1, JBCT2 Surface k - ε boundary condition types for the ξ and η directions.
- * JTBC1, JTBC2 Flags for type of time dependency for mean flow boundary conditions in the ξ and η directions.
- * KBC1, KBC2 Boundary types for the ξ and η directions.
- NBC Dimensioning parameter specifying number of boundary conditions per equation.
- NEQ Number of coupled equations being solved, N_{eq} .
- * NOUT Unit number for standard output.
- * NTBC Number of values in tables for general unsteady boundary conditions.
- * NTBCA Time levels at which general unsteady boundary conditions are specified.
- * N1, N2 Number of grid points N_1 and N_2 , in the ξ and η directions.

Output

- FBC1, FBC2 Point-by-point mean flow boundary condition values for the ξ and η directions.
- FBCT1, FBCT2 Point-by-point k - ε boundary condition values for the ξ and η directions.
- IBCELM Flags for elimination of off-diagonal coefficient submatrices resulting from three-point boundary conditions in the ξ and η directions at either boundary; 0 if elimination is not necessary, 1 if it is.

IBC1, IBC2	Point-by-point mean flow boundary condition types for the ξ and η directions.
IBCT1, IBCT2	Point-by-point k - ϵ boundary condition types for the ξ and η directions.
IBVUP	Flags for updating boundary values from first sweep after second sweep; 0 if updating is not necessary, 1 if it is.
JBC1, JBC2	Surface mean flow boundary condition types for the ξ and η directions (only if using the KBC meta flags.)
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .

Description

Subroutine BCSET sets various boundary condition parameters and flags. If boundary types are specified with the KBC meta flags, the appropriate surface boundary condition types are loaded into the JBC arrays. Special flags are set if spatially periodic boundary conditions are being used. BCSET also sets NPT1 and NPT2, the number of grid points in each ADI sweep direction to be used in computing coefficients and source terms. For spatially periodic boundary conditions in the ξ direction, $NPT1 = N1 + 1$. Similarly, for spatially periodic boundary conditions in the η direction, $NPT2 = N2 + 1$. This is done in order to use central differences at the periodic boundary. (See Section 7.2.2 of Volume 1.)

Next, if the boundary types are being specified using the KBC meta flags, the appropriate JBC mean flow boundary condition parameters are defined. Then, if the mean flow boundary conditions are being specified using the JBC and GBC parameters (or the KBC meta flags), the appropriate point-by-point boundary condition types and values (the IBC and FBC parameters) are loaded with the JBC and GBC values.

If three-point mean flow boundary conditions are being used at a boundary, a flag is set for eliminating the resulting off-diagonal coefficient submatrix. If gradient (two-point or three-point) or extrapolation mean flow boundary conditions are used during the first sweep, a flag is set for updating the ξ boundary values after the second sweep.

Next, for turbulent flow using the k - ϵ model, if the k - ϵ boundary conditions are being specified using the JBCT and GBCT parameters, the appropriate point-by-point boundary condition types and values (the IBCT and FBCT parameters) are loaded with the JBCT and GBCT values.

And finally, the input boundary condition parameters are then written to the standard output file.

Remarks

1. An error message is generated and execution is stopped if an invalid boundary type is specified with the KBC meta flags.

Subroutine BCTEMP (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMETS	Compute temperature boundary conditions.

Input

CP, CV	Specific heats c_p and c_v at time level n .
DEL	Computational grid spacing in sweep direction.
DTDRHO, DTDRU, DTDRV, DTDRW, DTDET	Derivatives $\partial T/\partial \rho$, $\partial T/\partial(\rho u)$, $\partial T/\partial(\rho v)$, $\partial T/\partial(\rho w)$, and $\partial T/\partial E_T$.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
* IHSTAG	Flag for constant stagnation enthalpy option.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i_v .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
P, T	Static pressure p and temperature T at time level n .
RGAS	Gas constant R .
RHO, U, V, W	Static density ρ , and velocities u , v , and w , at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCTEMP computes coefficients and source terms for temperature boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0

of Volume 1. The following sections apply these generalized equations to the particular temperature boundary conditions in *Proteus*.¹¹

No Change From Initial Conditions, $\Delta T = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{\mathbf{Q}} = J \partial g / \partial \mathbf{Q}$, we get simply

$$J_{i,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = 0$$

The derivatives $\partial T / \partial \rho$, $\partial T / \partial (\rho u)$, etc., depend on the equation of state. They are defined for a perfect gas in Section 4.3 of Volume 1.

Specified Static Temperature, $T = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = f_{i,j}^{n+1} - T_{i,j}^n$$

Specified Two-Point Temperature Gradient in Coordinate Direction, $\partial T / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -J_{1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\ & J_{2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\ & (\Delta \xi) f_{1,j}^{n+1} + T_{1,j}^n - T_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} & -J_{N_1-1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\ & J_{N_1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial (\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial (\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial (\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\ & (\Delta \xi) f_{N_1,j}^{n+1} + T_{N_1,j}^n - T_{N_1-1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Temperature Gradient in Coordinate Direction, $\partial T / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

¹¹ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n, representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& 2(\Delta \xi) f_{1,j}^{n+1} + 3T_{1,j}^n - 4T_{2,j}^n + T_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& 2(\Delta \xi) f_{N_1,j}^{n+1} - T_{N_1-2,j}^n + 4T_{N_1-1,j}^n - 3T_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Temperature Gradient in Normal Direction, $\nabla T \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned}
& -J_{1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& J_{2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n = \\
& \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta T_{1,j}^n \right] + T_{1,j}^n - T_{2,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& -J_{N_1-1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& J_{N_1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta T_{N_1,j}^n \right] + T_{N_1-1,j}^n - T_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Temperature Gradient in Normal Direction, $\nabla T \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned}
& -3J_{1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n + \\
& 4J_{2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n - \\
& J_{3,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
& \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta T_{1,j}^n \right] + 3T_{1,j}^n - 4T_{2,j}^n + T_{3,j}^n
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& J_{N_1-2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
& 4J_{N_1-1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
& 3J_{N_1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
& \frac{2\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta T_{N_1,j}^n \right] - T_{N_1-2,j}^n + 4T_{N_1-1,j}^n - 3T_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Static Temperature

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$\begin{aligned}
 & J_{1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{1,j}^n - \\
 & 2J_{2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{2,j}^n + \\
 & J_{3,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{3,j}^n = \\
 & -T_{1,j}^n + 2T_{2,j}^n - T_{3,j}^n
 \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
 & J_{N_1-2,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-2,j}^n - \\
 & 2J_{N_1-1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1-1,j}^n + \\
 & J_{N_1,j} \left[\frac{\partial T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T}{\partial E_T} \Delta \hat{E}_T \right]_{N_1,j}^n = \\
 & -T_{N_1-2,j}^n + 2T_{N_1-1,j}^n - T_{N_1,j}^n
 \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

No Change From Initial Conditions for Total Temperature, $\Delta T_T = 0$

The total temperature is defined as

$$T_T = T \left(1 + \frac{\gamma - 1}{2} M^2 \right)$$

Applying equation (6.3) of Volume 1, we get

$$J_{i,j} \left[\frac{\partial T_T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T_T}{\partial(\rho u)} \Delta(\hat{\rho} u) + \frac{\partial T_T}{\partial(\rho v)} \Delta(\hat{\rho} v) + \frac{\partial T_T}{\partial(\rho w)} \Delta(\hat{\rho} w) + \frac{\partial T_T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = 0$$

where

$$\begin{aligned}
\frac{\partial T_T}{\partial \rho} &= \frac{\partial T}{\partial \rho} \left(1 + \frac{\gamma-1}{2} M^2 \right) + \frac{\gamma-1}{2} T \frac{\partial M^2}{\partial \rho} \\
\frac{\partial T_T}{\partial(\rho u)} &= \frac{\partial T}{\partial(\rho u)} \left(1 + \frac{\gamma-1}{2} M^2 \right) + \frac{\gamma-1}{2} T \frac{\partial M^2}{\partial(\rho u)} \\
\frac{\partial T_T}{\partial(\rho v)} &= \frac{\partial T}{\partial(\rho v)} \left(1 + \frac{\gamma-1}{2} M^2 \right) + \frac{\gamma-1}{2} T \frac{\partial M^2}{\partial(\rho v)} \\
\frac{\partial T_T}{\partial(\rho w)} &= \frac{\partial T}{\partial(\rho w)} \left(1 + \frac{\gamma-1}{2} M^2 \right) + \frac{\gamma-1}{2} T \frac{\partial M^2}{\partial(\rho w)} \\
\frac{\partial T_T}{\partial E_T} &= \frac{\partial T}{\partial E_T} \left(1 + \frac{\gamma-1}{2} M^2 \right) + \frac{\gamma-1}{2} T \frac{\partial M^2}{\partial E_T}
\end{aligned}$$

The Mach number is defined by

$$M^2 = \frac{u^2 + v^2 + w^2}{\gamma R T} = \frac{(\rho u)^2 + (\rho v)^2 + (\rho w)^2}{\gamma R \rho^2 T}$$

The derivatives $\partial M^2 / \partial \rho$, etc., can then be derived as

$$\begin{aligned}
\frac{\partial M^2}{\partial \rho} &= -M^2 \left(\frac{2}{\rho} + \frac{1}{T} \frac{\partial T}{\partial \rho} \right) \\
\frac{\partial M^2}{\partial(\rho u)} &= \frac{2u}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho u)} \\
\frac{\partial M^2}{\partial(\rho v)} &= \frac{2v}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho v)} \\
\frac{\partial M^2}{\partial(\rho w)} &= \frac{2w}{\gamma p} - \frac{M^2}{T} \frac{\partial T}{\partial(\rho w)} \\
\frac{\partial M^2}{\partial E_T} &= -\frac{M^2}{T} \frac{\partial T}{\partial E_T}
\end{aligned}$$

Specified Total Temperature, $T_T = f$

Applying equation (6.5) of Volume 1, we get

$$\begin{aligned}
J_{i,j} \left[\frac{\partial T_T}{\partial \rho} \Delta \hat{\rho} + \frac{\partial T_T}{\partial(\rho u)} \Delta(\hat{\rho u}) + \frac{\partial T_T}{\partial(\rho v)} \Delta(\hat{\rho v}) + \frac{\partial T_T}{\partial(\rho w)} \Delta(\hat{\rho w}) + \frac{\partial T_T}{\partial E_T} \Delta \hat{E}_T \right]_{i,j}^n = \\
f_{i,j}^{n+1} - T_{i,j}^n \left(1 + \frac{\gamma-1}{2} M^2 \right)_{i,j}^n
\end{aligned}$$

where T_T , $\partial T_T / \partial \rho$, etc., are defined above as part of the description of the $\Delta T_T = 0$ boundary condition.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent temperature boundary condition is specified.

Subroutine BCUVEL (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute x-velocity boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i_v .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR, NRU	Array indices associated with the dependent variables ρ and ρu .
NVD, NPTSD	Leading two dimensions for the arrays A, P, C, and S.
RHO, U	Static density ρ and velocity u at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCUVEL computes coefficients and source terms for x-velocity boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular x-velocity boundary conditions in *Proteus*.¹²

¹² In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n , representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

No Change From Initial Conditions, $\Delta u = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{Q} = J \partial g / \partial Q$, we get simply

$$J_{i,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{i,j}^n = 0$$

Specified x-Velocity, $u = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{i,j}^n = f_{i,j}^{n+1} - u_{i,j}^n$$

Specified Two-Point x-Velocity Gradient in Coordinate Direction, $\partial u / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} -J_{1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{1,j}^n + J_{2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{2,j}^n = \\ (\Delta \xi) f_{1,j}^{n+1} + u_{1,j}^n - u_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} -J_{N_1-1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1,j}^n = \\ (\Delta \xi) f_{N_1,j}^{n+1} + u_{N_1-1,j}^n - u_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point x-Velocity Gradient in Coordinate Direction, $\partial u / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} -3J_{1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{2,j}^n - \\ J_{3,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{3,j}^n = 2(\Delta \xi) f_{1,j}^{n+1} + 3u_{1,j}^n - 4u_{2,j}^n + u_{3,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} J_{N_1-2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-1,j}^n + \\ 3J_{N_1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1,j}^n = 2(\Delta \xi) f_{N_1,j}^{n+1} - u_{N_1-2,j}^n + 4u_{N_1-1,j}^n - 3u_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point x-Velocity Gradient in Normal Direction, $\nabla u \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$-J_{1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{1,j}^n + J_{2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{2,j}^n =$$

$$\frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta u_{1,j}^n \right] + u_{1,j}^n - u_{2,j}^n$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$-J_{N_1-1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1,j}^n =$$

$$\frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta u_{N_1,j}^n \right] + u_{N_1-1,j}^n - u_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point x-Velocity Gradient in Normal Direction, $\nabla u \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$-3J_{1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{2,j}^n -$$

$$J_{3,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{3,j}^n = \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta u_{1,j}^n \right] +$$

$$3u_{1,j}^n - 4u_{2,j}^n + u_{3,j}^n$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-1,j}^n +$$

$$3J_{N_1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1,j}^n = \frac{2\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta u_{N_1,j}^n \right] -$$

$$u_{N_1-2,j}^n + 4u_{N_1-1,j}^n - 3u_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of x-Velocity

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$J_{1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{1,j}^n - 2J_{2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{2,j}^n + \\ J_{3,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{3,j}^n = -u_{1,j}^n + 2u_{2,j}^n - u_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-2,j}^n - 2J_{N_1-1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1-1,j}^n + \\ J_{N_1,j} \left[-\frac{u}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} u) \right]_{N_1,j}^n = -u_{N_1-2,j}^n + 2u_{N_1-1,j}^n - u_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent x -velocity boundary condition is specified.

Subroutine BCVDIR (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,METX,METY,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute normal and tangential velocity boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
J1	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
METX, METY	Derivatives of sweep direction computational coordinate with respect to x and y (or r if axisymmetric.)
* NOUT	Unit number for standard output.
NR, NRU, NRV, NRW	Array indices associated with the dependent variables ρ , ρu , ρv , and ρw .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, and METY.
NIP	Parameter specifying the dimension size in the ξ direction.
RHO, U, V, W	Static density ρ , and velocities u , v , and w , at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCVDIR computes coefficients and source terms for normal and tangential velocity boundary conditions. The linearized equations for the various general types of boundary conditions are

developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular normal and tangential velocity boundary conditions in *Proteus*.¹³

Specified Normal Velocity, $V_n = f$

The normal velocity is defined as

$$V_n = \vec{V} \cdot \vec{n}$$

where \vec{n} is the unit vector normal to the boundary. For a ξ boundary,

$$\vec{n} = \frac{\nabla \xi}{|\nabla \xi|} = \frac{1}{m} \xi_x \vec{i} + \frac{1}{m} \xi_y \vec{j}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

Therefore, for a ξ boundary,

$$V_n = \frac{1}{m} (\xi_x u + \xi_y v) = f$$

Note that the unit vector \vec{n} is in the direction of increasing ξ . Therefore V_n is positive in the direction of increasing ξ . Thus, a positive V_n at $\xi = 0$ implies flow into the computational domain, and a positive V_n at $\xi = 1$ implies flow out of the computational domain.

Similarly, for an η boundary,

$$V_n = \frac{1}{m} (\eta_x u + \eta_y v) = f$$

where

$$m = \sqrt{\eta_x^2 + \eta_y^2}$$

and V_n is positive in the direction of increasing η .

Applying equation (6.5) of Volume 1, the linearized boundary condition at a ξ boundary becomes

$$\frac{J_{i,j}}{m_{i,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{i,j}^n = f_{i,j}^{n+1} - (V_n)_{i,j}^n$$

An analogous equation can easily be written for the η boundaries.

¹³ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n, representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

Specified Two-Point Normal Velocity Gradient in Coordinate Direction, $\partial V_n / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$-\frac{J_{1,j}}{m_{1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n +$$

$$\frac{J_{2,j}}{m_{2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n =$$

$$(\Delta \xi) f_{1,j}^{n+1} + (V_n)_{1,j}^n - (V_n)_{2,j}^n$$

At the $\xi = 1$ boundary,

$$-\frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n +$$

$$\frac{J_{N_1,j}}{m_{N_1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n =$$

$$(\Delta \xi) f_{N_1,j}^{n+1} + (V_n)_{N_1-1,j}^n - (V_n)_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Normal Velocity Gradient in Coordinate Direction, $\partial V_n / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$-3 \frac{J_{1,j}}{m_{1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n +$$

$$4 \frac{J_{2,j}}{m_{2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n -$$

$$\frac{J_{3,j}}{m_{3,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n =$$

$$2(\Delta \xi) f_{1,j}^{n+1} + 3(V_n)_{1,j}^n - 4(V_n)_{2,j}^n + (V_n)_{3,j}^n$$

At the $\xi = 1$ boundary,

$$\frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n -$$

$$4 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n +$$

$$3 \frac{J_{N_1,j}}{m_{N_1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n =$$

$$2(\Delta \xi) f_{N_1,j}^{n+1} - (V_n)_{N_1-2,j}^n + 4(V_n)_{N_1-1,j}^n - 3(V_n)_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Normal Velocity Gradient in Normal Direction, $\nabla V_n \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -\frac{J_{1,j}}{m_{1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\ & \frac{J_{2,j}}{m_{2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n = \\ & \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta (V_n)_{1,j}^n \right] + (V_n)_{1,j}^n - (V_n)_{2,j}^n \end{aligned}$$

where δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} & -\frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\ & \frac{J_{N_1,j}}{m_{N_1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\ & \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta (V_n)_{N_1,j}^n \right] + (V_n)_{N_1-1,j}^n - (V_n)_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Normal Velocity Gradient in Normal Direction, $\nabla V_n \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} & -3 \frac{J_{1,j}}{m_{1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\ & 4 \frac{J_{2,j}}{m_{2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n - \\ & \frac{J_{3,j}}{m_{3,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n = \\ & \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta (V_n)_{1,j}^n \right] + 3(V_n)_{1,j}^n - 4(V_n)_{2,j}^n + (V_n)_{3,j}^n \end{aligned}$$

where δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& \frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n - \\
& 4 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\
& 3 \frac{J_{N_1,j}}{m_{N_1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\
& \frac{2\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta (V_n)_{N_1,j}^n \right] - (V_n)_{N_1-2,j}^n + 4(V_n)_{N_1-1,j}^n - 3(V_n)_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Normal Velocity

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$\begin{aligned}
& \frac{J_{1,j}}{m_{1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n - \\
& 2 \frac{J_{2,j}}{m_{2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n + \\
& \frac{J_{3,j}}{m_{3,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n = \\
& - (V_n)_{1,j}^n + 2(V_n)_{2,j}^n - (V_n)_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& \frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n - \\
& 2 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\
& \frac{J_{N_1,j}}{m_{N_1,j}} \left[-\frac{\xi_x u + \xi_y v}{\rho} \Delta \hat{\rho} + \frac{\xi_x}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_y}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\
& - (V_n)_{N_1-2,j}^n + 2(V_n)_{N_1-1,j}^n - (V_n)_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Tangential Velocity, $V_t = f$

For a ξ boundary, the tangential velocity is the velocity in the η direction, and is given by

$$\begin{aligned}
V_t = V_\eta &= \sqrt{u^2 + v^2 - V_n^2} \\
&= \frac{1}{m} (-\xi_y u + \xi_x v)
\end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

Note that this definition for tangential velocity does not include the swirl velocity w in axisymmetric flow. Separate boundary conditions should be set for w .

Similarly, for an η boundary,

$$V_t = V_\xi = \frac{1}{m} (\eta_y u - \eta_x v)$$

where

$$m = \sqrt{\eta_x^2 + \eta_y^2}$$

Applying equation (6.5) of Volume 1, the linearized boundary condition at a ξ boundary becomes

$$\frac{J_{i,j}}{m_{i,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{i,j}^n = f_{i,j}^{n+1} - (V_t)_{i,j}^n$$

An analogous equation can easily be written for the η boundaries.

Specified Two-Point Tangential Velocity Gradient in Coordinate Direction, $\partial V_t / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -\frac{J_{1,j}}{m_{1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\ & \frac{J_{2,j}}{m_{2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n = \\ & (\Delta \xi) f_{1,j}^{n+1} + (V_t)_{1,j}^n - (V_t)_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} & -\frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\ & \frac{J_{N_1,j}}{m_{N_1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\ & (\Delta \xi) f_{N_1,j}^{n+1} + (V_t)_{N_1-1,j}^n - (V_t)_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Tangential Velocity Gradient in Coordinate Direction, $\partial V_t / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned}
& -3 \frac{J_{1,j}}{m_{1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\
& 4 \frac{J_{2,j}}{m_{2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n - \\
& \frac{J_{3,j}}{m_{3,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n = \\
& 2(\Delta \xi) f_{1,j}^{n+1} + 3(V_D)_{1,j}^n - 4(V_D)_{2,j}^n + (V_D)_{3,j}^n
\end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& \frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n - \\
& 4 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\
& 3 \frac{J_{N_1,j}}{m_{N_1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\
& 2(\Delta \xi) f_{N_1,j}^{n+1} - (V_D)_{N_1-2,j}^n + 4(V_D)_{N_1-1,j}^n - 3(V_D)_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Tangential Velocity Gradient in Normal Direction, $\nabla V_i \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned}
& -\frac{J_{1,j}}{m_{1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\
& \frac{J_{2,j}}{m_{2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n = \\
& \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta (V_D)_{1,j}^n \right] + (V_D)_{1,j}^n - (V_D)_{2,j}^n
\end{aligned}$$

where δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned}
& -\frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\
& \frac{J_{N_1,j}}{m_{N_1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\
& \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta (V_D)_{N_1,j}^n \right] + (V_D)_{N_1-1,j}^n - (V_D)_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Tangential Velocity Gradient in Normal Direction, $\nabla V_t \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} & -3 \frac{J_{1,j}}{m_{1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n + \\ & 4 \frac{J_{2,j}}{m_{2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n - \\ & \frac{J_{3,j}}{m_{3,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n = \\ & \frac{2\Delta\xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta (V_t)_{1,j}^n \right] + 3(V_t)_{1,j}^n - 4(V_t)_{2,j}^n + (V_t)_{3,j}^n \end{aligned}$$

where δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} & \frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n - \\ & 4 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\ & 3 \frac{J_{N_1,j}}{m_{N_1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\ & \frac{2\Delta\xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta (V_t)_{N_1,j}^n \right] - (V_t)_{N_1-2,j}^n + 4(V_t)_{N_1-1,j}^n - 3(V_t)_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Tangential Velocity

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$\begin{aligned} & \frac{J_{1,j}}{m_{1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{1,j}^n - \\ & 2 \frac{J_{2,j}}{m_{2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{2,j}^n + \\ & \frac{J_{3,j}}{m_{3,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{3,j}^n = \\ & - (V_t)_{1,j}^n + 2(V_t)_{2,j}^n - (V_t)_{3,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned}
& \frac{J_{N_1-2,j}}{m_{N_1-2,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-2,j}^n - \\
& 2 \frac{J_{N_1-1,j}}{m_{N_1-1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1-1,j}^n + \\
& \frac{J_{N_1,j}}{m_{N_1,j}} \left[\frac{\xi_y u - \xi_x v}{\rho} \Delta \hat{\rho} - \frac{\xi_y}{\rho} \Delta(\hat{\rho} u) + \frac{\xi_x}{\rho} \Delta(\hat{\rho} v) \right]_{N_1,j}^n = \\
& - (V_\rho)_{N_1-2,j}^n + 2(V_\rho)_{N_1-1,j}^n - (V_\rho)_{N_1,j}^n
\end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent normal or tangential velocity boundary condition is specified.

Subroutine BCVVEL (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute y or r -velocity boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR, NRU, NRV	Array indices associated with the dependent variables ρ , ρu , and ρv .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
RHO, U, V	Static density ρ , and velocities u and v , at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCVVEL computes coefficients and source terms for y or r -velocity boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular y or r -velocity boundary conditions in *Proteus*.¹⁴

¹⁴ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n , representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

No Change From Initial Conditions, $\Delta v = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{\mathbf{Q}} = J \partial g / \partial \mathbf{Q}$, we get simply

$$J_{i,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{i,j}^n = 0$$

Specified y or r -Velocity, $v = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{i,j}^n = f_{i,j}^{n+1} - v_{i,j}^n$$

Specified Two-Point y or r -Velocity Gradient in Coordinate Direction, $\partial v / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} -J_{1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{1,j}^n + J_{2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{2,j}^n = \\ (\Delta \xi) f_{1,j}^{n+1} + v_{1,j}^n - v_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} -J_{N_1-1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1,j}^n = \\ (\Delta \xi) f_{N_1,j}^{n+1} + v_{N_1-1,j}^n - v_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point y or r -Velocity Gradient in Coordinate Direction, $\partial v / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} -3J_{1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{2,j}^n - \\ J_{3,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{3,j}^n = 2(\Delta \xi) f_{1,j}^{n+1} + 3v_{1,j}^n - 4v_{2,j}^n + v_{3,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} J_{N_1-2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-1,j}^n + \\ 3J_{N_1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1,j}^n = 2(\Delta \xi) f_{N_1,j}^{n+1} - v_{N_1-2,j}^n + 4v_{N_1-1,j}^n - 3v_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point y or r -Velocity Gradient in Normal Direction, $\nabla v \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} -J_{1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{1,j}^n + J_{2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{2,j}^n = \\ \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta v_{1,j}^n \right] + v_{1,j}^n - v_{2,j}^n \end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} -J_{N_1-1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1,j}^n = \\ \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta v_{N_1,j}^n \right] + v_{N_1-1,j}^n - v_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point y or r -Velocity Gradient in Normal Direction, $\nabla v \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} -3J_{1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{2,j}^n - \\ J_{3,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{3,j}^n = \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta v_{1,j}^n \right] + \\ 3v_{1,j}^n - 4v_{2,j}^n + v_{3,j}^n \end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} J_{N_1-2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-1,j}^n + \\ 3J_{N_1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1,j}^n = \frac{2\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta v_{N_1,j}^n \right] - \\ v_{N_1-2,j}^n + 4v_{N_1-1,j}^n - 3v_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of y or r -Velocity

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$J_{1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{1,j}^n - 2J_{2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{2,j}^n + \\ J_{3,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{3,j}^n = -v_{1,j}^n + 2v_{2,j}^n - v_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-2,j}^n - 2J_{N_1-1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1-1,j}^n + \\ J_{N_1,j} \left[-\frac{v}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho}v) \right]_{N_1,j}^n = -v_{N_1-2,j}^n + 2v_{N_1-1,j}^n - v_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Flow Angle, $\tan^{-1}(v/u) = f$

This boundary condition can be rewritten as

$$\frac{v}{u} = \tan f$$

where f is the specified flow angle. Multiplying by ρu ,

$$(\tan f)\rho u - \rho v = 0$$

Applying equation (6.5) of Volume 1 to the above equation, we get

$$J_{i,j} \left[(\tan f)_{i,j}^{n+1} \Delta(\hat{\rho}u)_{i,j}^n - \Delta(\hat{\rho}v)_{i,j}^n \right] = -(\tan f)_{i,j}^n + (\rho v)_{i,j}^n$$

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent y -velocity boundary condition is specified.

Subroutine BCWVEL (IBC,FBC,IEQ,IMIN,IMAX,IBOUND,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BCGEN	BCGRAD BCMET	Compute swirl velocity boundary conditions.

Input

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
IBC, FBC	Mean flow boundary condition types and values for current sweep direction, specified as IBC(I,J) and FBC(I,J), where I runs from 1 to N_{eq} , corresponding to the N_{eq} conditions needed, and J = 1 or 2, corresponding to the lower and upper boundaries.
IBOUND	Flag specifying boundary; 1 for lower boundary, 2 for upper boundary.
IEQ	Boundary condition equation number.
IMIN, IMAX	Minimum and maximum indices in the sweep direction.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i_v .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
* NOUT	Unit number for standard output.
NR, NRU, NRW	Array indices associated with the dependent variables ρ , ρu , and ρw .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
RHO, U, W	Static density ρ , and velocities u and w , at time level n .

Output

A, B, C	Coefficient submatrices A, B, and C at boundary IBOUND (row IEQ only).
S	Source term subvector S at boundary IBOUND (element IEQ only).

Description

Subroutine BCWVEL computes coefficients and source terms for swirl velocity boundary conditions. The linearized equations for the various general types of boundary conditions are developed in Section 6.0 of Volume 1. The following sections apply these generalized equations to the particular swirl velocity boundary conditions in *Proteus*.¹⁵

¹⁵ In the following description, for the first ADI sweep the dependent variables should have the superscript *, representing the intermediate solution, and for the second ADI sweep they should have the superscript n , representing the final solution. For simplicity, however, only the superscript n is used. The superscripts on all other variables are correct as written.

No Change From Initial Conditions, $\Delta w = 0$

Applying equation (6.3) of Volume 1, and noting that $\partial g / \partial \hat{Q} = J \partial g / \partial Q$, we get simply

$$J_{i,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{i,j}^n = 0$$

Specified Swirl Velocity, $w = f$

Applying equation (6.5) of Volume 1,

$$J_{i,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{i,j}^n = f_{i,j}^{n+1} - w_{i,j}^n$$

Specified Two-Point Swirl Velocity Gradient in Coordinate Direction, $\partial w / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} -J_{1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{1,j}^n + J_{2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{2,j}^n = \\ (\Delta \xi) f_{1,j}^{n+1} + w_{1,j}^n - w_{2,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} -J_{N_1-1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{N_1,j}^n = \\ (\Delta \xi) f_{N_1,j}^{n+1} + w_{N_1-1,j}^n - w_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Swirl Velocity Gradient in Coordinate Direction, $\partial w / \partial \phi = f$

Applying equation (6.8) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} -3J_{1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{2,j}^n - \\ J_{3,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{3,j}^n = 2(\Delta \xi) f_{1,j}^{n+1} + 3w_{1,j}^n - 4w_{2,j}^n + w_{3,j}^n \end{aligned}$$

At the $\xi = 1$ boundary,

$$\begin{aligned} J_{N_1-2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{N_1-1,j}^n + \\ 3J_{N_1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\rho \hat{w}) \right]_{N_1,j}^n = 2(\Delta \xi) f_{N_1,j}^{n+1} - w_{N_1-2,j}^n + 4w_{N_1-1,j}^n - 3w_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Two-Point Swirl Velocity Gradient in Normal Direction, $\nabla \mathbf{w} \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using two-point one-sided differencing,

$$\begin{aligned} & -J_{1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{1,j}^n + J_{2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{2,j}^n = \\ & \frac{\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta w_{1,j}^n \right] + w_{1,j}^n - w_{2,j}^n \end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} & -J_{N_1-1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1-1,j}^n + J_{N_1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1,j}^n = \\ & \frac{\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta w_{N_1,j}^n \right] + w_{N_1-1,j}^n - w_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Specified Three-Point Swirl Velocity Gradient in Normal Direction, $\nabla \mathbf{w} \cdot \vec{n} = f$

Applying equation (6.12a) of Volume 1 at the $\xi = 0$ boundary, and using three-point one-sided differencing,

$$\begin{aligned} & -3J_{1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{1,j}^n + 4J_{2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{2,j}^n - \\ & J_{3,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{3,j}^n = \frac{2\Delta \xi}{m_{1,j}} \left[f_{1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{1,j}}{m_{1,j}} \delta_\eta w_{1,j}^n \right] + \\ & 3w_{1,j}^n - 4w_{2,j}^n + w_{3,j}^n \end{aligned}$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

and δ_η is the centered difference operator presented in Section 5.0 of Volume 1. At the $\xi = 1$ boundary,

$$\begin{aligned} & J_{N_1-2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1-2,j}^n - 4J_{N_1-1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1-1,j}^n + \\ & 3J_{N_1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1,j}^n = \frac{2\Delta \xi}{m_{N_1,j}} \left[f_{N_1,j}^{n+1} - \frac{(\xi_x \eta_x + \xi_y \eta_y)_{N_1,j}}{m_{N_1,j}} \delta_\eta w_{N_1,j}^n \right] - \\ & w_{N_1-2,j}^n + 4w_{N_1-1,j}^n - 3w_{N_1,j}^n \end{aligned}$$

Analogous equations can easily be written for the η boundaries.

Linear Extrapolation of Swirl Velocity

Applying equation (6.14) of Volume 1 at the $\xi = 0$ boundary,

$$J_{1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{1,j}^n - 2J_{2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{2,j}^n + \\ J_{3,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{3,j}^n = -w_{1,j}^n + 2w_{2,j}^n - w_{3,j}^n$$

At the $\xi = 1$ boundary,

$$J_{N_1-2,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1-2,j}^n - 2J_{N_1-1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1-1,j}^n + \\ J_{N_1,j} \left[-\frac{w}{\rho} \Delta \hat{\rho} + \frac{1}{\rho} \Delta(\hat{\rho} w) \right]_{N_1,j}^n = -w_{N_1-2,j}^n + 2w_{N_1-1,j}^n - w_{N_1,j}^n$$

Analogous equations can easily be written for the η boundaries.

Specified Flow Angle, $\tan^{-1}(w/u) = f$

This boundary condition can be rewritten as

$$\frac{w}{u} = \tan f$$

where f is the specified flow angle. Multiplying by ρu ,

$$(\tan f) \rho u - \rho w = 0$$

Applying equation (6.5) of Volume 1 to the above equation, we get

$$J_{i,j} \left[(\tan f)_{i,j}^{n+1} \Delta(\hat{\rho} u)_{i,j}^n - \Delta(\hat{\rho} w)_{i,j}^n \right] = -(\tan f)_{i,j}^n + (\rho w)_{i,j}^n$$

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. An error message is generated and execution is stopped if a non-existent swirl velocity boundary condition is specified.

Subroutine BLIN1		
Called by	Calls	Purpose
TURBBL	ISRCHEQ	Compute inner layer turbulent viscosity along constant ξ lines.

Input

* APLUS	Van Driest damping constant A^+ .
* CB	Constant B in the Spalding-Kleinstein inner layer model.
* CNL	Exponent n in the Launder-Priddin modified mixing length formula for the inner region of the Baldwin-Lomax turbulence model.
* CVK	Von Karman mixing length constant used in the inner region of the Baldwin-Lomax and Spalding-Kleinstein models.
* IDEBUG	Debug flags.
* ILDAMP	Flag for Launder-Priddin modified mixing length formula in the Baldwin-Lomax inner region model.
* INNER	Flag for type of inner region model.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
IT	Current time step number n .
* IWALL2	Flags indicating whether or not the η boundaries are walls.
II	Grid index i in the ξ direction.
* LWALL2	Flags specifying wall locations for η boundaries.
MU	Laminar coefficient of viscosity μ_l .
MUT	Outer layer turbulent viscosity coefficient $(\mu_t)_{out}$ along constant ξ lines.
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
* N2	Number of grid points N_2 in the η direction.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w .
VORT	Total vorticity magnitude.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

MUT	Turbulent viscosity coefficient μ_t along constant ξ lines.
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Description

Subroutine BLIN1 computes the inner layer turbulent viscosity coefficient $(\mu_t)_{inner}$ at a specified ξ location (i.e., due to walls at $\eta = 0$ and/or $\eta = 1$.) Two different inner region models are available - the model of Baldwin and Lomax (1978), and the model of Spalding (1961) and Kleinstein (1967). These are described in Section 9.1.2 of Volume 1.

If both η boundaries are solid walls, $(\mu_t)_{inner}$ is computed separately for each wall, and it is assumed that the two inner regions do not overlap. For each wall, the computation is done inside a loop starting at the wall and moving outward. Once the inner region value exceeds the outer region value, the loop is exited. Thus $\mu_t = (\mu_t)_{inner}$ until $(\mu_t)_{inner} \geq (\mu_t)_{outer}$, then $\mu_t = (\mu_t)_{outer}$.

The distribution of μ_t across the intersection of the inner and outer regions is smoothed using the following formulas. For the $\eta = 0$ wall,

$$\begin{aligned}(\mu_t)_{j_b} &= \frac{1}{4} [(\mu_t)_{j_b-1} + 2(\mu_t)_{j_b} + (\mu_t)_{j_b+1}] \\(\mu_t)_{j_b-1} &= \frac{1}{4} [(\mu_t)_{j_b-2} + 2(\mu_t)_{j_b-1} + (\mu_t)_{j_b}]\end{aligned}$$

where the boundary between the inner and outer regions falls between $j = j_b - 1$ and $j = j_b$. It should be noted that the unsmoothed value of $(\mu_t)_{j_b}$ is used in the second smoothing formula, not the smoothed value from the first formula. Similarly, for the $\eta = 1$ wall,

$$\begin{aligned}(\mu_t)_{j_b} &= \frac{1}{4} [(\mu_t)_{j_b+1} + 2(\mu_t)_{j_b} + (\mu_t)_{j_b-1}] \\(\mu_t)_{j_b+1} &= \frac{1}{4} [(\mu_t)_{j_b+2} + 2(\mu_t)_{j_b+1} + (\mu_t)_{j_b}]\end{aligned}$$

where the boundary between the inner and outer regions falls between $j = j_b + 1$ and $j = j_b$.

Remarks

1. To avoid the possibility of floating point errors, the value of $|\bar{\Omega}|_w$ used to compute τ^+ and u^+ is set to a minimum of 10^{-10} .
2. The Cray search routine ISRCHEQ is used in determining the grid locations for debug printout.
3. This subroutine generates output for the IDEBUG(8) option.

Subroutine BLIN2		
Called by	Calls	Purpose
TURBBL	ISRCHEQ	Compute inner layer turbulent viscosity along constant η lines.

Input

* APLUS	Van Driest damping constant A^+ .
* CB	Constant B in the Spalding-Kleinstein inner layer model.
* CNL	Exponent n in the Launder-Priddin modified mixing length formula for the inner region of the Baldwin-Lomax turbulence model.
* CVK	Von Karman mixing length constant used in the inner region of the Baldwin-Lomax and Spalding-Kleinstein models.
DUMMY	Outer layer turbulent viscosity coefficient $(\mu_t)_{outer}$ along constant η lines.
* IDEBUG	Debug flags.
* ILDAMP	Flag for Launder-Priddin modified mixing length formula in the Baldwin-Lomax inner region model.
* INNER	Flag for type of inner region model.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
IT	Current time step number n .
* IWALL1	Flags indicating whether or not the ξ boundaries are walls.
I2	Grid index j in the η direction.
* LWALL1	Flags specifying wall locations for ξ boundaries.
MU	Laminar coefficient of viscosity μ_l .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
* N1	Number of grid points N_1 in the ξ direction.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w .
VORT	Total vorticity magnitude.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

DUMMY	Turbulent viscosity coefficient μ_t along constant η lines.
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Description

Subroutine BLIN2 computes the inner layer turbulent viscosity coefficient $(\mu_t)_{inner}$ at a specified η location (i.e., due to walls at $\xi = 0$ and/or $\xi = 1$.) The procedure is exactly analogous to that used in subroutine BLIN1.

Subroutine BLKOUT (I1PT,I2PT,A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI AVISC1 AVISC2 BCGEN FILTER		Print coefficient blocks at specified indices in the ξ and η directions.

Input

A, B, C	Coefficient submatrices A, B, and C
* IHSTAG	Flag for constant stagnation enthalpy option.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
I1PT, I2PT	Indices for printout in the ξ and η directions.
NC, NXM, NYM, NZM, NEN	Array indices associated with the continuity, x -momentum, y -momentum (or r -momentum if axisymmetric), swirl momentum, and energy equations.
NEQ	Number of coupled equations being solved, N_{eq} .
* NOUT	Unit number for standard output.
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

None.

Description

Subroutine BLKOUT prints the coefficient block submatrices A, B, and C, and the source term subvector S at the grid points specified by I1PT and I2PT. This is the routine that actually prints the output for the IDEBUG(1) through IDEBUG(4) options.

Subroutine BLK2 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXECT		Solve 2×2 block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK2 solves a block tridiagonal system of equations with 2×2 blocks using the block matrix version of the Thomas algorithm. The algorithm is described in Section 7.2.1 of Volume 1. For clarity, that description involves additional "new" matrices \mathbf{D} , \mathbf{E} , and $\Delta\hat{\mathbf{Q}}'$. In Fortran, however, we can save storage by overwriting B, C, and S. The following table relates the algorithm as implemented in Fortran to the notation used in Volume 1, for the first ADI sweep. An exactly analogous procedure is followed for the second sweep.

Step	In Fortran	In Volume 1 Notation
1		$\mathbf{D}_2 = \mathbf{B}_2$
2a	Solve $\mathbf{B}_2\mathbf{E}_2 = \mathbf{C}_1$ for \mathbf{E}_2 , storing result in \mathbf{C}_2	$\mathbf{E}_2 = \mathbf{D}_2^{-1}\mathbf{C}_2$
2b	Solve $\mathbf{B}_2\Delta\hat{\mathbf{Q}}'_2 = \mathbf{S}_2$ for $\Delta\hat{\mathbf{Q}}'_2$, storing result in \mathbf{S}_2	$\Delta\hat{\mathbf{Q}}'_2 = \mathbf{D}_2^{-1}\mathbf{S}_2$
3a	For $i = 3$ to $N_1 - 1$, Compute $\mathbf{B}_i - \mathbf{A}_i\mathbf{C}_{i-1}$, storing result in \mathbf{B}_i	$\mathbf{D}_i = \mathbf{B}_i - \mathbf{A}_i\mathbf{E}_{i-1}$
3b	Compute $\mathbf{S}_i - \mathbf{A}_i\mathbf{S}_{i-1}$, storing result in \mathbf{S}_i	$\mathbf{S}_i - \mathbf{A}_i\Delta\hat{\mathbf{Q}}'_{i-1}$
3c	Solve $\mathbf{B}_i\mathbf{E}_i = \mathbf{C}_i$ for \mathbf{E}_i , storing result in \mathbf{C}_i	$\mathbf{E}_i = \mathbf{D}_i^{-1}\mathbf{C}_i$
3d	Solve $\mathbf{B}_i\Delta\hat{\mathbf{Q}}'_i = \mathbf{S}_i$ for $\Delta\hat{\mathbf{Q}}'_i$, storing result in \mathbf{S}_i	$\Delta\hat{\mathbf{Q}}'_i = \mathbf{D}_i^{-1}(\mathbf{S}_i - \mathbf{A}_i\Delta\hat{\mathbf{Q}}'_{i-1})$
4		$\Delta\hat{\mathbf{Q}}'_{N_1-1} = \Delta\hat{\mathbf{Q}}'_{N_1-1}$
5	For $i = N_1 - 2$ to 2 , Compute $\mathbf{S}_i - \mathbf{C}_i\mathbf{S}_{i+1}$, storing result in \mathbf{S}_i	$\Delta\hat{\mathbf{Q}}_i = \Delta\hat{\mathbf{Q}}'_i - \mathbf{E}_i\Delta\hat{\mathbf{Q}}'_{i+1}$

Remarks

1. The notation used in the comments in BLK2 is consistent with the notation used in the description of the algorithm in Volume 1. However, BLK2 is actually used to solve the k - ϵ turbulence model equations, and the boundary conditions for these equations are treated explicitly. That's why the index in BLK2 runs from $i = 2$ to $N_1 - 1$, instead of from $i = 1$ to N_1 . In addition, in BLK2 the matrix \mathbf{D}^{-1} is computed directly, rather than by LU decomposition.

2. The Thomas algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK2P (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXECT		Solve 2×2 periodic block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK2P solves a periodic block tridiagonal system of equations with 2×2 blocks. An efficient algorithm similar to the block matrix version of the Thomas algorithm is used to solve the equations. The algorithm is described in Section 7.2.2 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, **F**, **G**, and $\Delta\hat{Q}'$. In Fortran, however, we can save storage by overwriting A, B, C, and S. The following table relates the algorithm as implemented in Fortran to the notation used in Volume 1, for the first ADI sweep. An exactly analogous procedure is followed for the second sweep.

Step	In Fortran	In Volume 1 Notation
1a 1b		$D_2 = B_2$ $F_2 = C_{N_1}$
2a 2b 2c	Solve $B_2 E_2 = C_2$ for E_2 , storing result in C_2 Solve $B_2 G_2 = A_2$ for G_2 , storing result in A_2 Solve $B_2 \Delta\hat{Q}'_2 = S_2$ for $\Delta\hat{Q}'_2$, storing result in S_2	$E_2 = D_2^{-1} C_2$ $G_2 = D_2^{-1} A_2$ $\Delta\hat{Q}'_2 = D_2^{-1} S_2$
3a 3b 3c 3d 3e 3f 3g 3h 3i	For $i = 3$ to $N_1 - 1$, Compute $B_i - A_i C_{i-1}$, storing result in B_i Compute $S_i - A_i S_{i-1}$, storing result in S_i Compute $-A_i A_{i-1}$, storing result in A_i Solve $B_i E_i = C_i$ for E_i , storing result in C_i Solve $B_i G_i = A_i$ for G_i , storing result in A_i Solve $B_i \Delta\hat{Q}'_i = S_i$ for $\Delta\hat{Q}'_i$, storing result in S_i Compute $B_{N_1} - C_{N_1} A_{i-1}$, storing result in B_{N_1} Compute $S_{N_1} - C_{N_1} S_{i-1}$, storing result in S_{N_1} Compute $-C_{N_1} C_{i-1}$, storing result in C_{N_1}	$D_i = B_i - A_i E_{i-1}$ $S_i - A_i \Delta\hat{Q}'_{i-1}$ $- A_i G_{i-1}$ $E_i = D_i^{-1} C_i$ $G_i = D_i^{-1} A_i G_{i-1}$ $\Delta\hat{Q}'_i = D_i^{-1} (S_i - A_i \Delta\hat{Q}'_{i-1})$ $B_{N_1} - \sum_{j=2}^{i-1} F_j G_j$ $S_{N_1} - \sum_{j=2}^{i-1} F_j \Delta\hat{Q}'_j$ $F_i = -F_{i-1} E_{i-1}$

Step	In Fortran	In Volume 1 Notation
4a	Compute $A_{N_1-1} + C_{N_1-1}$, storing result in A_{N_1-1}	$G_{N_1-1} = D_{N_1-1}^{-1}(C_{N_1-1} - A_{N_1-1}G_{N_1-2})$
4b	Compute $A_{N_1} + C_{N_1}$, storing result in C_{N_1}	$F_{N_1-1} = A_{N_1} - F_{N_1-2}E_{N_1-2}$
4c	Compute $B_{N_1} - C_{N_1}A_{N_1-1}$, storing result in B_{N_1}	$D_{N_1} = B_{N_1} - \sum_{i=2}^{N_1-1} F_i G_i$
4d	Compute $S_{N_1} - C_{N_1}S_{N_1-1}$, storing result in S_{N_1}	$S_{N_1} - \sum_{i=2}^{N_1-1} F_i \Delta \hat{Q}'_i$
4f	Solve $B_{N_1} \Delta \hat{Q}'_{N_1} = S_{N_1}$ for $\Delta \hat{Q}'_{N_1}$, storing result in S_{N_1}	$\Delta \hat{Q}'_{N_1} = D_{N_1}^{-1}(S_{N_1} - \sum_{i=2}^{N_1-1} F_i \Delta \hat{Q}'_i)$
5		$\Delta \hat{Q}_{N_1} = \Delta \hat{Q}'_{N_1}$
6	Compute $S_{N_1-1} - A_{N_1-1}S_{N_1}$, storing result in S_{N_1-1}	$\Delta \hat{Q}'_{N_1-1} = \Delta \hat{Q}'_{N_1-1} - G_{N_1-1} \Delta \hat{Q}_{N_1}$
7	For $i = N_1 - 2$ to 2, Compute $S_i - A_i S_{N_1} - C_i S_{i+1}$, storing result in S_i	$\Delta \hat{Q}_i = \Delta \hat{Q}'_i - G_i \Delta \hat{Q}_{N_1} - E_i \Delta \hat{Q}_{i+1}$
8	Set $S_1 = S_{N_1}$	$\Delta \hat{Q}_1 = \Delta \hat{Q}_{N_1}$

Remarks

1. The notation used in the comments in BLK2P is consistent with the notation used in the description of the algorithm in Volume 1. However, in BLK2P the matrix D^{-1} is computed directly, rather than by LU decomposition.
2. The solution algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK3 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI	FILTER	Solve 3×3 block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK3 solves a block tridiagonal system of equations with 3×3 blocks using the block matrix version of the Thomas algorithm. Subroutine FILTER is called in an attempt to eliminate any zero values on the diagonal of the submatrix **B** at the two boundaries. These can occur when mean flow boundary conditions are specified using the JBC and/or IBC input parameters, depending on the initial conditions and the order of the boundary conditions.

The algorithm is described in Section 7.2.1 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, and $\hat{\Delta Q}'$. In Fortran, however, storage is saved by overwriting B, C, and S. The following table relates the algorithm as implemented in Fortran to the notation used in Volume 1, for the first ADI sweep. An exactly analogous procedure is followed for the second sweep.

Step	In Fortran	In Volume 1 Notation
1		$D_1 = B_1$
2a	LU decompose B_1 , storing result in B_1	LU decomposition of D_1
2b	Solve $B_1 E_1 = C_1$ for E_1 using LU decomposition of B_1 , storing result in C_1	$E_1 = D_1^{-1} C_1$
2c	Solve $B_1 \Delta \hat{Q}'_1 = S_1$ for $\Delta \hat{Q}'_1$ using LU decomposition of B_1 , storing result in S_1	$\Delta \hat{Q}'_1 = D_1^{-1} S_1$
3a	For $i = 2$ to N_1 , Compute $B_i - A_i C_{i-1}$, storing result in B_i	$D_i = B_i - A_i E_{i-1}$
3b	Compute $S_i - A_i S_{i-1}$, storing result in S_i	$S_i - A_i \Delta \hat{Q}'_{i-1}$
3c	LU decompose B_i , storing result in B_i	LU decomposition of D_i
3d	Solve $B_i E_i = C_i$ for E_i using LU decomposition of B_i , storing result in C_i	$E_i = D_i^{-1} C_i$
3e	Solve $B_i \Delta \hat{Q}'_i = S_i$ for $\Delta \hat{Q}'_i$ using LU decomposition of B_i , storing result in S_i	$\Delta \hat{Q}'_i = D_i^{-1} (S_i - A_i \Delta \hat{Q}'_{i-1})$
4		$\Delta \hat{Q}'_{N_1} = \Delta \hat{Q}'_{N_1}$

Step	In Fortran	In Volume 1 Notation
5	For $i = N_1 - 1$ to 1, Compute $S_i - C_i S_{i+1}$, storing result in S_i	$\Delta \hat{Q}_i = \Delta \hat{Q}'_i - E_i \Delta \hat{Q}_{i-1}$

Remarks

1. The notation used in the comments in BLK3 is consistent with the notation used in the description of the algorithm in Volume 1.
2. The Thomas algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK3P (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI		Solve 3×3 periodic block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A , B , and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A , B , C , and S .
S	Source term subvector S .

Output

S	Computed solution subvector.
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Description

Subroutine BLK3P solves a periodic block tridiagonal system of equations with 3×3 blocks. An efficient algorithm similar to the block matrix version of the Thomas algorithm is used to solve the equations. The algorithm is described in Section 7.2.2 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, **F**, **G**, and $\Delta\hat{Q}'$. In Fortran, however, storage is saved by overwriting **A**, **B**, **C**, and **S**. The following table relates the algorithm as implemented in Fortran to the notation used in Volume 1, for the first ADI sweep. An exactly analogous procedure is followed for the second sweep.

Step	In Fortran	In Volume 1 Notation
1a		$\mathbf{D}_2 = \mathbf{B}_2$
1b		$\mathbf{F}_2 = \mathbf{C}_{N_1}$
2a	LU decompose \mathbf{B}_2 , storing result in \mathbf{B}_2	LU decomposition of \mathbf{D}_2
2b	Solve $\mathbf{B}_2\mathbf{E}_2 = \mathbf{C}_2$ for \mathbf{E}_2 using LU decomposition of \mathbf{B}_2 , storing result in \mathbf{C}_2	$\mathbf{E}_2 = \mathbf{D}_2^{-1}\mathbf{C}_2$
2c	Solve $\mathbf{B}_2\mathbf{G}_2 = \mathbf{A}_2$ for \mathbf{G}_2 using LU decomposition of \mathbf{B}_2 , storing result in \mathbf{A}_2	$\mathbf{G}_2 = \mathbf{D}_2^{-1}\mathbf{A}_2$
2d	Solve $\mathbf{B}_2\Delta\hat{Q}'_2 = \mathbf{S}_2$ for $\Delta\hat{Q}'_2$ using LU decomposition of \mathbf{B}_2 , storing result in \mathbf{S}_2	$\Delta\hat{Q}'_2 = \mathbf{D}_2^{-1}\mathbf{S}_2$

Step	In Fortran	In Volume 1 Notation
	For $i = 3$ to $N_1 - 1$,	
3a	Compute $B_i - A_i C_{i-1}$, storing result in B_i	$D_i = B_i - A_i E_{i-1}$
3b	Compute $S_i - A_i S_{i-1}$, storing result in S_i	$S_i - A_i \Delta \hat{Q}'_{i-1}$
3c	Compute $-A_i A_{i-1}$, storing result in A_i	$-A_i G_{i-1}$
3d	LU decompose B_i , storing result in B_i	LU decomposition of D_i
3e	Solve $B_i E_i = C_i$ for E_i using LU decomposition of B_i , storing result in C_i	$E_i = D_i^{-1} C_i$
3f	Solve $B_i G_i = A_i$ for G_i using LU decomposition of B_i , storing result in A_i	$G_i = D_i^{-1} A_i G_{i-1}$
3g	Solve $B_i \Delta \hat{Q}'_i = S_i$ for $\Delta \hat{Q}'_i$ using LU decomposition of B_i , storing result in S_i	$\Delta \hat{Q}'_i = D_i^{-1} (S_i - A_i \Delta \hat{Q}'_{i-1})$
3h	Compute $B_{N_1} - C_{N_1} A_{i-1}$, storing result in B_{N_1}	$B_{N_1} - \sum_{j=2}^{i-1} F_j G_j$
3i	Compute $S_{N_1} - C_{N_1} S_{i-1}$, storing result in S_{N_1}	$S_{N_1} - \sum_{j=2}^{i-1} F_j \Delta \hat{Q}'_j$
3j	Compute $-C_{N_1} C_{i-1}$, storing result in C_{N_1}	$F_i = -F_{i-1} E_{i-1}$
4a	Compute $A_{N_1-1} + C_{N_1-1}$, storing result in A_{N_1-1}	$G_{N_1-1} = D_{N_1-1}^{-1} (C_{N_1-1} - A_{N_1-1} G_{N_1-2})$
4b	Compute $A_{N_1} + C_{N_1}$, storing result in C_{N_1}	$F_{N_1-1} = A_{N_1} - F_{N_1-2} E_{N_1-2}$
4c	Compute $B_{N_1} - C_{N_1} A_{N_1-1}$, storing result in B_{N_1}	$D_{N_1} = B_{N_1} - \sum_{i=2}^{N_1-1} F_i G_i$
4d	Compute $S_{N_1} - C_{N_1} S_{N_1-1}$, storing result in S_{N_1}	$S_{N_1} - \sum_{i=2}^{N_1-1} F_i \Delta \hat{Q}'_i$
4e	LU decompose B_{N_1} , storing result in B_{N_1}	LU decomposition of D_{N_1}
4f	Solve $B_{N_1} \Delta \hat{Q}'_{N_1} = S_{N_1}$ for $\Delta \hat{Q}'_{N_1}$ using LU decomposition of B_{N_1} , storing result in S_{N_1}	$\Delta \hat{Q}'_{N_1} = D_{N_1}^{-1} (S_{N_1} - \sum_{i=2}^{N_1-1} F_i \Delta \hat{Q}'_i)$
5		$\Delta \hat{Q}_{N_1} = \Delta \hat{Q}'_{N_1}$
6	Compute $S_{N_1-1} - A_{N_1-1} S_{N_1}$, storing result in S_{N_1-1}	$\Delta \hat{Q}_{N_1-1} = \Delta \hat{Q}'_{N_1-1} - G_{N_1-1} \Delta \hat{Q}_{N_1}$
	For $i = N_1 - 2$ to 2 ,	
7	Compute $S_i - A_i S_{N_1} - C_i S_{i+1}$, storing result in S_i	$\Delta \hat{Q}_i = \Delta \hat{Q}'_i - G_i \Delta \hat{Q}_{N_1} - E_i \Delta \hat{Q}_{i+1}$
8	Set $S_1 = S_{N_1}$	$\Delta \hat{Q}_1 = \Delta \hat{Q}_{N_1}$

Remarks

1. The notation used in the comments in BLK3P is consistent with the notation used in the description of the algorithm in Volume 1.
2. The solution algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK4 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI	FILTER	Solve 4×4 block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK4 solves a block tridiagonal system of equations with 4×4 blocks using the block matrix version of the Thomas algorithm. Subroutine FILTER is called in an attempt to eliminate any zero values on the diagonal of the submatrix **B** at the two boundaries. These can occur when mean flow boundary conditions are specified using the JBC and/or IBC input parameters, depending on the initial conditions and the order of the boundary conditions.

The algorithm is described in Section 7.2.1 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, and $\Delta\hat{Q}'$. In Fortran, however, storage is saved by overwriting B, C, and S. The algorithm is identical to that used in subroutine BLK3. See the description of that subroutine for a table relating the algorithm as implemented in Fortran to the notation used in Volume 1.

Remarks

1. The notation used in the comments in BLK4 is consistent with the notation used in the description of the algorithm in Volume 1.
2. The Thomas algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK4P (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI		Solve 4×4 periodic block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK4P solves a periodic block tridiagonal system of equations with 4×4 blocks. An efficient algorithm similar to the block matrix version of the Thomas algorithm is used to solve the equations. The algorithm is described in Section 7.2.2 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, **F**, **G**, and $\Delta\hat{Q}'$. In Fortran, however, storage is saved by overwriting A, B, C, and S. The algorithm is identical to that used in subroutine BLK3P. See the description of that subroutine for a table relating the algorithm as implemented in Fortran to the notation used in Volume 1.

Remarks

1. The notation used in the comments in BLK4P is consistent with the notation used in the description of the algorithm in Volume 1.
2. The solution algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK5 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI	FILTER	Solve 5×5 block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK5 solves a block tridiagonal system of equations with 5×5 blocks using the block matrix version of the Thomas algorithm. Subroutine FILTER is called in an attempt to eliminate any zero values on the diagonal of the submatrix **B** at the two boundaries. These can occur when mean flow boundary conditions are specified using the JBC and/or IBC input parameters, depending on the initial conditions and the order of the boundary conditions.

The algorithm is described in Section 7.2.1 of Volume 1. For clarity, that description involves additional "new" matrices **D**, **E**, and $\Delta\hat{Q}'$. In Fortran, however, storage is saved by overwriting B, C, and S. The algorithm is identical to that used in subroutine BLK3. See the description of that subroutine for a table relating the algorithm as implemented in Fortran to the notation used in Volume 1.

Remarks

1. The notation used in the comments in BLK5 is consistent with the notation used in the description of the algorithm in Volume 1.
2. The Thomas algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

Subroutine BLK5P (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
ADI		Solve 5×5 periodic block tridiagonal system of equations.

Input

A, B, C	Coefficient submatrices A, B, and C
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S.

Output

S	Computed solution subvector.
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Description

Subroutine BLK5P solves a periodic block tridiagonal system of equations with 5×5 blocks. An efficient algorithm similar to the block matrix version of the Thomas algorithm is used to solve the equations. The algorithm is described in Section 7.2.2 of Volume 1. For clarity, that description involves additional "new" matrices D, E, F, G, and $\Delta\hat{Q}'$. In Fortran, however, storage is saved by overwriting A, B, C, and S. The algorithm is identical to that used in subroutine BLK3P. See the description of that subroutine for a table relating the algorithm as implemented in Fortran to the notation used in Volume 1.

Remarks

1. The notation used in the comments in BLK5P is consistent with the notation used in the description of the algorithm in Volume 1.
2. The solution algorithm is recursive and therefore cannot be vectorized in the sweep direction. In an ADI procedure, however, if the coefficients and source terms are stored in both directions, the algorithm can be vectorized in the non-sweep direction. That is the reason for the first, or IV, subscript on the A, B, C, and S arrays. It was added simply to allow vectorization of the BLK routines. This increases the storage required by the program, but greatly decreases the CPU time required for the ADI solution.

BLOCK DATA Subprogram		
Called by	Calls	Purpose
		Set default values for input parameters, plus a few other parameters.

Input

None.

Output

All namelist input parameters, plus:

CCP1, CCP2, CCP3, CCP4	Constants in formula for specific heat. $(8.53 \times 10^3, 3.12 \times 10^4, 2.065 \times 10^6, 7.83 \times 10^8)^{16}$
CK1, CK2	Constants in formula for laminar thermal conductivity coefficient. $(7.4907 \times 10^{-3}, 350.0)^{16}$
CMU1, CMU2	Constants in formula for laminar viscosity coefficient. $(7.3035 \times 10^{-7}, 198.6)^{16}$
GC	Proportionality factor g_c in Newton's second law. $(32.174)^{16}$
IBCELM	Flags for elimination of off-diagonal coefficient submatrices resulting from three-point boundary conditions in the ξ and η directions at either boundary; 0 if elimination is not necessary, 1 if it is. $(2*0, 2*0)$
IBVUP	Flags for updating boundary values from first sweep after second sweep; 0 if updating is not necessary, 1 if it is. $(0,0)$
ICONV	Convergence flag; 1 if converged, 0 if not. (0)
IGINT	Flags for grid interpolation requirement for the ξ and η directions; 0 if interpolation is not necessary, 1 if it is. $(0,0)$
ITBEG	The time level n at the beginning of a run. (1)
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic. $(0,0)$
NC, NXM, NYM, NZM, NEN	Array indices associated with the continuity, x -momentum, y -momentum (or r -momentum if axisymmetric), swirl momentum, and energy equations. $(1,2,3,5,4)$
NIN	Unit number for standard input. (5)
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T . $(1,2,3,5,4)$
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow. $(NMAXP*1.0)$
TAU	Initial time value τ . $(NTOTP*0.0)$

¹⁶ These values are for reference conditions specified in English units. Values for SI units are set in subroutine INPUT.

Description

The BLOCK DATA routine is used to set default values for all the input parameters, plus various other parameters and constants. The defaults for all the input parameters are given as part of the standard input description in Section 3.1 of Volume 2. The values for the other parameters and constants set in BLOCK DATA are given in parentheses in the above output description. Note that some of these values assume English units are being used to specify reference conditions. If SI units are being used, these values are re-defined in subroutine INPUT.

Remarks

1. Most of the default values are defined directly, but some, like the reference viscosity MUR, are set equal to zero and defined in subroutine INPUT if not specified by the user.

Subroutine BLOUT1		
Called by	Calls	Purpose
TURBBL	ISAMAX ISAMIN ISRCHEQ	Compute outer layer turbulent viscosity, using the algebraic Baldwin-Lomax model, along constant ξ lines.

Input

* APLUS	Van Driest damping constant A^+ .
* CB	Constant B in the Klebanoff intermittency factor.
* CCLAU	Clauser constant K in the Baldwin-Lomax outer region model.
* CCP	Constant C_{cp} in the Baldwin-Lomax outer region model.
* CKLEB, CKMIN	Constants C_{Kleb} and $(C_{Kleb})_{min}$ in the Klebanoff intermittency factor.
* CNA	Exponent n in the formula used to average the two outer region μ_t profiles that result when both boundaries in a coordinate direction are solid surfaces.
* CWK	Constant C_{wk} in the Baldwin-Lomax outer region model.
* IDEBUG	Debug flags.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
IT	Current time step number n .
* IWALL2	Flags indicating whether or not the η boundaries are walls.
II	Grid index i in the ξ direction.
* LWALL2	Flags specifying wall locations for η boundaries.
MU	Laminar coefficient of viscosity μ_l .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
* N2	Number of grid points N_2 in the η direction.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w .
VORT	Total vorticity magnitude.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

LWAKE2	Grid index j in the η direction used as the origin for computing length scales for free turbulent flows.
MUT	Outer layer turbulent viscosity coefficient $(\mu_t)_{outer}$ along constant ξ lines.

Description

Subroutine BLOUT1 computes the outer layer turbulent viscosity coefficient $(\mu_t)_{outer}$ at a specified ξ location (i.e., due to walls at $\eta = 0$ and/or $\eta = 1$, or due to a free turbulent flow in the ξ direction) using the

algebraic eddy viscosity model of Baldwin and Lomax (1978). The model is described in Section 9.1 of Volume 1. The steps performed in BLOUT1 are as follows:

1. Find the values and locations of $|\vec{V}|_{max}$ and $|\vec{V}|_{min}$.
2. Compute the parameter

$$F_{wake} = \begin{cases} y_{max} F_{max} & \text{for wall-bounded flows} \\ C_{wk} V_{diff}^2 \frac{y_{max}}{F_{max}} & \text{for free turbulent flows} \end{cases}$$

where C_{wk} is a constant taken as 0.25, and

$$V_{diff} = |\vec{V}|_{max} - |\vec{V}|_{min}$$

where \vec{V} is the total velocity vector. The procedure for computing the parameter F_{max} depends on whether a solid wall exists at $\eta = 0$ and/or at $\eta = 1$.

3. If, at the current ξ location, the $\eta = 0$ boundary is a solid wall, compute $(F_{max})_1$ as follows:

- 3a. For η -indices from the wall to the location of $|\vec{V}|_{max}$, compute

$$F(y_n) = y_n |\vec{\Omega}| \left(1 - e^{-y^+/A^+}\right)$$

- 3b. Get the location of the maximum value of $F(y_n)$, calling its η -index L_1 . Tentatively set $(L_{max})_1 = L_1$.
- 3c. Search outward from this location for a local minimum in $F(y_n)$. If one is found, call its η -index L_{min} .
- 3d. If a local minimum exists, get the location of the next maximum value of $F(y_n)$, calling its η -index L_2 . This is the location of the second peak in $F(y_n)$. Let

$$\Delta F_1 = F(y_n)_{L_1} - F(y_n)_{L_{min}}$$

$$\Delta F_2 = F(y_n)_{L_2} - F(y_n)_{L_{min}}$$

Then, if $\Delta F_2 > 0.25 \Delta F_1$, set $(L_{max})_1 = L_2$. This test is intended to filter false peaks resulting from noise, or wiggles, in $F(y_n)$.

- 3e. Set $(F_{max})_1 = F(y_n)$ at the η -index $(L_{max})_1$, and set y_{max} equal to the corresponding value of y_n .
4. If, at the current ξ location, the $\eta = 1$ boundary is a solid wall, compute $(F_{max})_2$. The procedure is exactly analogous to the procedure described in steps 3a-3e for computing $(F_{max})_1$ at the $\eta = 0$ wall.
5. If neither η boundary is a solid wall, a free turbulent flow in the ξ direction is assumed. In this case, the required value of F_{max} is computed as follows:
 - 5a. For η -indices between the locations of $|\vec{V}|_{min}$ and $|\vec{V}|_{max}$, and using the location of $|\vec{V}|_{max}$ as the origin for y_n , compute

$$F(y_n) = y_n |\vec{\Omega}|$$

Get the location of the maximum value of $F(y_n)$, and compute F_{wake} .

- 5b. Repeat step 5a using the location of $|\vec{V}|_{min}$ as the origin for y_n .
- 5c. Set the final value of F_{wake} equal to the one from step 5a or 5b that corresponds to the smaller value of y_{max} . Set L_{wake} accordingly.

6. If a solid wall exists at $\eta = 0$ or at $\eta = 1$, but not both, or if neither η boundary is a solid wall, compute $(\mu_t)_{outer}$ directly.
7. If both η boundaries are solid walls, compute $(\mu_t)_{outer}$ by combining the two computed values of F_{wake} using the averaging formula presented as equation (9.12) of Volume 1.

Remarks

1. The computation of y_n , the normal distance to the wall or wake centerline, is approximate. It is actually the straight-line distance between the interior grid point and the wall or wake centerline grid point.
2. The Cray search routines ISAMAX and ISAMIN are used in computing $|\bar{V}_{max}|$, $|\bar{V}_{min}|$, and F_{max} . The Cray search routine ISRCHEQ is used in determining the grid locations for debug printout.
3. If the maximum and minimum total velocities are equal, indicating a uniform flow along this particular ξ line, their locations are arbitrarily set equal to the middle η index, and the turbulent viscosity coefficient $(\mu_t)_{outer}$ is set equal to 0. This normally would occur only during the first time step in a case with uniform initial velocity profiles.
4. To avoid the possibility of floating point errors, the values of $|\bar{V}_{max}|$, $|\bar{V}_{min}|$, F_{max} , and y_{max} are set to a minimum of 10^{-10} .
5. This subroutine generates output for the IDEBUG(8) option.

Subroutine BLOUT2		
Called by	Calls	Purpose
TURBBL	ISAMAX ISAMIN ISRCHEQ	Compute outer layer turbulent viscosity, using the algebraic Baldwin-Lomax model, along constant η lines.

Input

* APLUS	Van Driest damping constant A^+ .
* CB	Constant B in the Klebanoff intermittency factor.
* CCLAU	Clauser constant K in the Baldwin-Lomax outer region model.
* CCP	Constant C_{cp} in the Baldwin-Lomax outer region model.
* CKLEB, CKMIN	Constants C_{Kleb} and $(C_{Kleb})_{min}$ in the Klebanoff intermittency factor.
* CNA	Exponent n in the formula used to average the two outer region μ_t profiles that result when both boundaries in a coordinate direction are solid surfaces.
* CWK	Constant C_{wk} in the Baldwin-Lomax outer region model.
* IDEBUG	Debug flags.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
IT	Current time step number n .
* IWALL1	Flags indicating whether or not the ξ boundaries are walls.
I2	Grid index j in the η direction.
* LWALL1	Flags specifying wall locations for ξ boundaries.
MU	Laminar coefficient of viscosity μ_l .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
* N1	Number of grid points N_1 in the ξ direction.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w .
VORT	Total vorticity magnitude.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

LWAKEI	Grid index i in the ξ direction used as the origin for computing length scales for free turbulent flows.
DUMMY	Outer layer turbulent viscosity coefficient $(\mu_t)_{outer}$ along constant η lines.

Description

Subroutine BLOUT2 computes the outer layer turbulent viscosity coefficient $(\mu_t)_{outer}$ at a specified η location (i.e., due to walls at $\xi = 0$ and/or $\xi = 1$, or due to a free turbulent flow in the η direction) using the

algebraic eddy viscosity model of Baldwin and Lomax (1978). The procedure is exactly analogous to that used in subroutine BLOUT1.

Subroutine BVUP (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	BCGEN EQSTAT SGEFA SGESL	Update first sweep boundary values after second sweep.

Input

A, B, C	Coefficient submatrices A, B, and C.
DXI	Computational grid spacing $\Delta\xi$.
IBVUP	Flags for updating boundary values from first sweep after second sweep; 0 if updating is not necessary, 1 if it is.
* IHSTAG	Flag for constant stagnation enthalpy option.
* ISWIRL	Flag for swirl in axisymmetric flow.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
NEQ	Number of coupled equations being solved, N_{eq} .
NEQP	Dimensioning parameter specifying maximum number of coupled equations allowed.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
N1P	Parameter specifying the dimension size in the ξ direction.
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n at all grid points.
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level $n + 1$ at all interior grid points.
S	Source term subvector S.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .

Output

DEL	Computational grid spacing for the sweep direction being updated.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
ISWEEP	ADI sweep number for sweep direction being updated.
IV	Index in the "vectorized" direction, i_v .
METX, METY, METT	Derivatives of computational coordinate, for the sweep direction being updated, with respect to x , y (or r if axisymmetric), and t .

NPTS	Number of grid points N in the sweep direction being updated.
NV	Number of grid points in the "vectorized" direction, N_v .
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level $n + 1$ at boundary points from first sweep.

Description

Subroutine BVUP updates boundary values from the first, or ξ , sweep after the second, or η , sweep. In general, this is necessary when gradient or extrapolation boundary conditions are used in the ξ direction. Some updating is also necessary when spatially periodic boundary conditions are used. The procedure is described in Section 7.3 of Volume 1 for all cases.

Remarks

1. The corner values of ρ and E_T are updated by linearly extrapolating from the two adjacent points in the ξ and η directions, and averaging the two results. Note that this extrapolation is done in computational space. Grid packing in either direction is thus not taken into account. The corner values of the velocities are updated by doing the same type of extrapolation. Instead of averaging, however, the extrapolated velocity whose absolute value is lower is used. This was done to maintain no-slip at duct inlets and exits.
2. Subroutines SGEFA and SGESL are Cray LINPACK routines. In general terms, if the Fortran arrays A and S represent A and S, where A is a square N by N matrix and S is a vector with N elements, and if the leading dimension of the Fortran array A is LDA, then the Fortran sequence

```
call sgefa (a,lda,n,ipvt,info)
call sgesl (a,lda,n,ipvt,s,0)
```

computes $A^{-1}S$, storing the result in S.

Subroutine COEFC (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Compute coefficients and source term for the continuity equation.

Input

DEL	Computational grid spacing in sweep direction.
DTAU	Time step $\Delta\tau$.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* IAXI	Flag for axisymmetric flow.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IHSTAG	Flag for constant stagnation enthalpy option.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} (times the radius r for axisymmetric flow.)
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
NC	Array index associated with the continuity equation.
NEQ	Number of coupled equations being solved, N_{eq} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, METY, and METT.
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow.
RHO, U, V	Static density ρ , and velocities u and v , at time level n .
RHOL	Static density ρ from previous ADI sweep.
* THC	Parameters θ_1 and θ_2 determining type of time differencing for the continuity equation.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .
Y	Radial coordinate r for axisymmetric flow.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points (row NC only).
---------	---

Description

Subroutine COEFC computes the coefficients and source term for the continuity equation. Equations (7.5a-b) in Volume 1 represent, in vector form, the four governing difference equations for the two ADI sweeps for 2-D planar flow. The elements of the inviscid flux vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{F}}$ are given in Section 2.0 of Volume 1, and the elements of the viscous flux vectors $\hat{\mathbf{E}}_{v1}$, $\hat{\mathbf{E}}_{v2}$, etc., are given in Appendix A of Volume 1. The Jacobian coefficient matrices $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$, $\partial\hat{\mathbf{E}}_{v1}/\partial\hat{\mathbf{Q}}$, etc., are given in Section 4.0 of Volume 1. Using all of these equations, the differenced form of the continuity equation for 2-D planar flow may be written for the two ADI sweeps as¹⁷

Sweep 1 (ξ direction)

$$\Delta\hat{\rho}_i^* + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi} \left[\left(\frac{\partial\hat{\mathbf{E}}_1}{\partial\hat{\mathbf{Q}}} \right)_{i+1}^n \Delta\hat{\mathbf{Q}}_{i+1}^* - \left(\frac{\partial\hat{\mathbf{E}}_1}{\partial\hat{\mathbf{Q}}} \right)_{i-1}^n \Delta\hat{\mathbf{Q}}_{i-1}^* \right] =$$

$$- \frac{\Delta\tau}{1+\theta_2} (\delta_\xi\hat{\mathbf{E}}_1 + \delta_\eta\hat{\mathbf{F}}_1)^n + \frac{\theta_2}{1+\theta_2} \Delta\hat{\rho}^{n-1}$$

Sweep 2 (η direction)

$$\Delta\hat{\rho}_j^n + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\eta} \left[\left(\frac{\partial\hat{\mathbf{F}}_1}{\partial\hat{\mathbf{Q}}} \right)_{j+1}^n \Delta\hat{\mathbf{Q}}_{j+1}^n - \left(\frac{\partial\hat{\mathbf{F}}_1}{\partial\hat{\mathbf{Q}}} \right)_{j-1}^n \Delta\hat{\mathbf{Q}}_{j-1}^n \right] = \Delta\hat{\rho}^*$$

In the above equations, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j .

The vector of dependent variables is

$$\hat{\mathbf{Q}} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad E_T]^T$$

The appropriate elements of the flux vectors are given by

$$\hat{\mathbf{E}}_1 = \frac{1}{J} [\rho u \xi_x + \rho v \xi_y + \rho \xi_t]$$

$$\hat{\mathbf{F}}_1 = \frac{1}{J} [\rho u \eta_x + \rho v \eta_y + \rho \eta_t]$$

The elements of the Jacobian coefficient matrix $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$ for the continuity equation are

$$\frac{\partial\hat{\mathbf{E}}_1}{\partial\hat{\mathbf{Q}}} = [\xi_t \quad \xi_x \quad \xi_y \quad 0]$$

¹⁷ These equations are written assuming the energy equation is being solved. For a constant stagnation enthalpy case, the total energy E_T would not appear as a dependent variable, and the Jacobian coefficient matrices would have only three elements.

The Jacobian coefficient matrix $\partial \hat{\mathbf{F}}_1 / \partial \hat{\mathbf{Q}}$ has the same form as $\partial \hat{\mathbf{E}}_1 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

As an example of how these equations are translated into Fortran, consider the $\Delta(\rho u/J)$ term on the left hand side for the first sweep. This is the second element of $\hat{\mathbf{Q}}$, so using the second element in $\partial \hat{\mathbf{E}}_1 / \partial \hat{\mathbf{Q}}$ we get

$$\begin{aligned} A(\text{IV}, \text{I}, \text{NC}, \text{NRU}) &= -\frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} (\xi_x)_{i-1,j} \\ B(\text{IV}, \text{I}, \text{NC}, \text{NRU}) &= 0 \\ C(\text{IV}, \text{I}, \text{NC}, \text{NRU}) &= \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} (\xi_x)_{i+1,j} \end{aligned}$$

The equations for axisymmetric flow are developed in Appendix B of Volume 1. The axisymmetric continuity equation for the two ADI sweeps is given by¹⁸

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta \hat{\rho}_i^* + \frac{\theta_1 \Delta\tau}{(1+\theta_2)2\Delta\xi} \frac{1}{r} \left[\left(r \frac{\partial \hat{\mathbf{E}}_1}{\partial \hat{\mathbf{Q}}} \right)_{i+1}^n \Delta \hat{\mathbf{Q}}_{i+1}^* - \left(r \frac{\partial \hat{\mathbf{E}}_1}{\partial \hat{\mathbf{Q}}} \right)_{i-1}^n \Delta \hat{\mathbf{Q}}_{i-1}^* \right] = \\ - \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} [\delta_\xi(r \hat{\mathbf{E}}_1) + \delta_\eta(r \hat{\mathbf{F}}_1)]^n + \frac{\theta_2}{1+\theta_2} \Delta \hat{\rho}^{n-1} \end{aligned}$$

Sweep 2 (η direction)

$$\Delta \hat{\rho}_j^n + \frac{\theta_1 \Delta\tau}{(1+\theta_2)2\Delta\eta} \frac{1}{r} \left[\left(r \frac{\partial \hat{\mathbf{F}}_1}{\partial \hat{\mathbf{Q}}} \right)_{j+1}^n \Delta \hat{\mathbf{Q}}_{j+1}^n - \left(r \frac{\partial \hat{\mathbf{F}}_1}{\partial \hat{\mathbf{Q}}} \right)_{j-1}^n \Delta \hat{\mathbf{Q}}_{j-1}^n \right] = \Delta \hat{\rho}^*$$

where now

$$\begin{aligned} \hat{\mathbf{Q}} &= \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T \\ \hat{\mathbf{E}}_1 &= \frac{1}{J} [\rho u \xi_x + \rho v \xi_r + \rho \xi_t] \\ \hat{\mathbf{F}}_1 &= \frac{1}{J} [\rho u \eta_x + \rho v \eta_r + \rho \eta_t] \\ \frac{\partial \hat{\mathbf{E}}_1}{\partial \hat{\mathbf{Q}}} &= [\xi_r \quad \xi_x \quad \xi_r \quad 0 \quad 0] \end{aligned}$$

As in 2-D planar flow, the Jacobian coefficient matrix $\partial \hat{\mathbf{F}}_1 / \partial \hat{\mathbf{Q}}$ has the same form as $\partial \hat{\mathbf{E}}_1 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

¹⁸ These equations are written for the general case with swirl. For a non-swirl case, the swirl momentum ρw would not appear as a dependent variable, and the Jacobian coefficient matrices would have only four elements.

Note that the equations for 2-D planar and axisymmetric flow are very similar. In the axisymmetric equations, the radius r appears as an additional coefficient in front of the flux vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{F}}$, and in front of the Jacobian coefficient matrices $\partial \hat{\mathbf{E}}_1 / \partial \hat{\mathbf{Q}}$ and $\partial \hat{\mathbf{F}}_1 / \partial \hat{\mathbf{Q}}$. In addition, $1/r$ appears in front of every term in the equation except the $\Delta \hat{\rho}$ terms. In *Proteus*, the Fortran variables are defined in such a way that, for many terms, the same coding can be used for both 2-D planar and axisymmetric flow. Unfortunately, this may make some of the coding a little confusing. It is hoped that this detailed description, when compared with the source listing, will help make things clear.

In COEFC, the coefficients of the left hand side, or implicit, terms are defined first. The implicit terms for the second ADI sweep have exactly the same form as for the first sweep, but with ξ replaced by η . By defining DEL, METX, METY, and METT as the grid spacing and metric coefficients in the sweep direction, the same coding can be used for both sweeps. The variable RAX is equal to 1 for 2-D planar flow, and the radius r for axisymmetric flow. This adds the r in front of the Jacobian coefficient matrices for axisymmetric flow, but has no effect for 2-D planar flow. The $1/r$ coefficient in front of each term will be added later. In this section of code, the coefficient of $\Delta \hat{\rho}$ (part of B(IV,I,NC,NR)) is set equal to r , not 1 as it should be. This will be corrected later.

The source term, or right hand side, for the first sweep is defined next. The difference formulas used to compute the source term are the same as those used for the implicit terms. These formulas are presented in Section 5.0 of Volume 1. For axisymmetric flow, the Fortran variable JI, which is normally defined as $1/J$, is temporarily redefined as r/J before the COEF routines are called. This automatically accounts for the r coefficient in front of all the flux vectors in the source term. The $1/r$ coefficient in front of each term will be added later. This definition of JI adds an r in front of the $\Delta \hat{\rho}^{n-1}$ term that should not be there. This will also be corrected later.

The coding for the source term for the second sweep, which consists only of $\Delta \hat{\rho}^*$, comes next. The definition of JI also adds an r in front of this term that should not be there.

And finally, for axisymmetric flow, the entire equation is divided by the local radius r . This adds the $1/r$ coefficient where it should be added, and removes the r in front of the $\Delta \hat{\rho}$ terms.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For sections of the code that apply to both sweeps (i.e., the implicit terms and the division by r at the end), the first two subscripts are written as (IV,I). For sections of the code that apply only to the first sweep, the first two subscripts are written as (I2,I1). For sections that apply only to the second sweep, they are written as (I1,I2). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.

Subroutine COEFE (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Compute coefficients and source term for the energy equation.

Input

DEL	Computational grid spacing in sweep direction.
DPDRHO, DPDRU, DPDRV, DPDRW, DPDET	Derivatives $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, $\partial p/\partial(\rho v)$, $\partial p/\partial(\rho w)$, and $\partial p/\partial E_T$.
DTAU	Time step $\Delta \tau$.
DTDRHO, DTDRU, DTDRV, DTDRW, DTDET	Derivatives $\partial T/\partial \rho$, $\partial T/\partial(\rho u)$, $\partial T/\partial(\rho v)$, $\partial T/\partial(\rho w)$, and $\partial T/\partial E_T$.
DXI, DETA	Computational grid spacing $\Delta \xi$ and $\Delta \eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_z .
* IAXI	Flag for axisymmetric flow.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IEULER	Flag for Euler calculation.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
* ITHIN	Flags for thin-layer option.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} (times the radius r for axisymmetric flow.)
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
MU, LA, KT	Effective coefficient of viscosity μ , effective second coefficient of viscosity λ , and effective coefficient of thermal conductivity k at time level n .
NEN	Array index associated with the energy equation.
NEQ	Number of coupled equations being solved, N_{eq} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, METY, and METT.
P, T	Static pressure p and temperature T at time level n .
PRR	Reference Prandtl number Pr_r .
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow.
* RER	Reference Reynolds number Re_r .

RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
* THE	Parameters θ_1 , θ_2 , and θ_3 determining type of time differencing for the energy equation.
TL	Static temperature T from previous ADI sweep.
UL, VL, WL, ETL	Velocities u , v , and w , and total energy E_T from previous ADI sweep.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ , if axisymmetric), and ξ_r .
Y	Radial coordinate r for axisymmetric flow.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points (row NEN only).
S	Source term subvector S at interior points (element NEN only).

Description

Subroutine COEFE computes the coefficients and source term for the energy equation. Equations (7.5a-b) in Volume 1 represent, in vector form, the four governing difference equations for the two ADI sweeps for 2-D planar flow. The elements of the inviscid flux vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{F}}$ are given in Section 2.0 of Volume 1, and the elements of the viscous flux vectors $\hat{\mathbf{E}}_{v_1}$, $\hat{\mathbf{E}}_{v_2}$, etc., are given in Appendix A of Volume 1. The Jacobian coefficient matrices $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$, $\partial\hat{\mathbf{E}}_{v_1}/\partial\hat{\mathbf{Q}}$, etc., are given in Section 4.0 of Volume 1. Using all of these equations, the differenced form of the energy equation for 2-D planar flow may be written for the two ADI sweeps as

Sweep 1 (ξ direction)

$$\begin{aligned}
\Delta(\hat{E}_T)_i^* + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \xi} & \left[\left(\frac{\partial \hat{\mathbf{E}}_4}{\partial \hat{\mathbf{Q}}} \right)_{i+1}^n \Delta \hat{\mathbf{Q}}_{i+1}^* - \left(\frac{\partial \hat{\mathbf{E}}_4}{\partial \hat{\mathbf{Q}}} \right)_{i-1}^n \Delta \hat{\mathbf{Q}}_{i-1}^* \right] \\
& - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \xi)^2} \left[(f_{i-1} + f_i)^n g_{i-1}^n \Delta \hat{\mathbf{Q}}_{i-1}^* - (f_{i-1} + 2f_i + f_{i+1})^n g_i^n \Delta \hat{\mathbf{Q}}_i^* + (f_i + f_{i+1})^n g_{i+1}^n \Delta \hat{\mathbf{Q}}_{i+1}^* \right] = \\
& - \frac{\Delta \tau}{1 + \theta_2} (\delta_\xi \hat{\mathbf{E}}_4 + \delta_\eta \hat{\mathbf{F}}_4)^n + \frac{\Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{v_1})_4 + \delta_\eta (\hat{\mathbf{F}}_{v_1})_4]^n \\
& + \frac{(1 + \theta_3) \Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{v_2})_4 + \delta_\eta (\hat{\mathbf{F}}_{v_2})_4]^n - \frac{\theta_3 \Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{v_2})_4 + \delta_\eta (\hat{\mathbf{F}}_{v_2})_4]^{n-1} + \frac{\theta_2}{1 + \theta_2} \Delta \hat{E}_T^{n-1}
\end{aligned}$$

Sweep 2 (η direction)

$$\Delta(\hat{E}_T)_j^n + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \eta} \left[\left(\frac{\partial \hat{F}_4}{\partial \hat{Q}} \right)_{j+1}^n \Delta \hat{Q}_{j+1}^n - \left(\frac{\partial \hat{F}_4}{\partial \hat{Q}} \right)_{j-1}^n \Delta \hat{Q}_{j-1}^n \right] \\ - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \eta)^2} \left[(f_{j-1} + f_j)^n g_{j-1}^n \Delta \hat{Q}_{j-1}^n - (f_{j-1} + 2f_j + f_{j+1})^n g_j^n \Delta \hat{Q}_j^n + (f_j + f_{j+1})^n g_{j+1}^n \Delta \hat{Q}_{j+1}^n \right] = \\ \Delta \hat{E}_T^*$$

In the above equations, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j . On the left hand side, f is the coefficient of $\partial/\partial \xi$ (or $\partial/\partial \eta$, depending on the sweep) in the $\partial \hat{E}_{v1}/\partial \hat{Q}$ (or $\partial \hat{F}_{v1}/\partial \hat{Q}$) Jacobian coefficient matrix. Similarly, g is the term in the parentheses following $\partial/\partial \xi$ (or $\partial/\partial \eta$) in the $\partial \hat{E}_{v1}/\partial \hat{Q}$ (or $\partial \hat{F}_{v1}/\partial \hat{Q}$) Jacobian coefficient matrix.

The vector of dependent variables is

$$\hat{Q} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad E_T]^T$$

The appropriate elements of the inviscid flux vectors are given by

$$\hat{E}_4 = \frac{1}{J} [(E_T + p)u\xi_x + (E_T + p)v\xi_y + E_T \xi_t] \\ \hat{F}_4 = \frac{1}{J} [(E_T + p)u\eta_x + (E_T + p)v\eta_y + E_T \eta_t]$$

The appropriate elements of the non-cross derivative viscous flux vectors are

$$(\hat{E}_{v1})_4 = \frac{1}{J} \frac{1}{Re_r} \left\{ \frac{(2\mu + \lambda)}{2} [\xi_x^2 (u^2)_\xi + \xi_y^2 (v^2)_\xi] + (\mu + \lambda) \xi_x \xi_y (uv)_\xi \right. \\ \left. + \frac{\mu}{2} [\xi_x^2 (v^2)_\xi + \xi_y^2 (u^2)_\xi] + \frac{k}{Pr_r} (\xi_x^2 + \xi_y^2) T_\xi \right\} \\ (\hat{F}_{v1})_4 = \frac{1}{J} \frac{1}{Re_r} \left\{ \frac{(2\mu + \lambda)}{2} [\eta_x^2 (u^2)_\eta + \eta_y^2 (v^2)_\eta] + (\mu + \lambda) \eta_x \eta_y (uv)_\eta \right. \\ \left. + \frac{\mu}{2} [\eta_x^2 (v^2)_\eta + \eta_y^2 (u^2)_\eta] + \frac{k}{Pr_r} (\eta_x^2 + \eta_y^2) T_\eta \right\}$$

And the appropriate elements of the cross derivative viscous flux vectors are

$$(\hat{E}_{v2})_4 = \frac{1}{J} \frac{1}{Re_r} \left[2\mu (\xi_x \eta_x u u_\eta + \xi_y \eta_y v v_\eta) + \lambda \xi_x (\eta_x u u_\eta + \eta_y u v_\eta) + \lambda \xi_y (\eta_x v u_\eta + \eta_y v v_\eta) \right. \\ \left. + \mu \xi_x (\eta_y v u_\eta + \eta_x v v_\eta) + \mu \xi_y (\eta_y u u_\eta + \eta_x u v_\eta) + \frac{k}{Pr_r} (\xi_x \eta_x + \xi_y \eta_y) T_\eta \right]$$

$$(\hat{\mathbf{F}}_{\nu_2})_4 = \frac{1}{J} \frac{1}{Re_r} \left[2\mu(\eta_x \xi_x u u_\xi + \eta_y \xi_y v v_\xi) + \lambda \eta_x (\xi_x u u_\xi + \xi_y u v_\xi) + \lambda \eta_y (\xi_x v u_\xi + \xi_y v v_\xi) \right. \\ \left. + \mu \eta_x (\xi_y v u_\xi + \xi_x v v_\xi) + \mu \eta_y (\xi_y u u_\xi + \xi_x u v_\xi) + \frac{k}{Pr_r} (\eta_x \xi_x + \eta_y \xi_y) T_\xi \right]$$

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}} / \partial \hat{\mathbf{Q}}$ for the inviscid terms in the energy equation are

$$\frac{\partial \hat{\mathbf{E}}_4}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} -f_1 \left(f_2 - \frac{\partial p}{\partial \rho} \right) & f_2 \xi_x + f_1 \frac{\partial p}{\partial(\rho u)} & f_2 \xi_y + f_1 \frac{\partial p}{\partial(\rho v)} & \xi_t + f_1 \left(1 + \frac{\partial p}{\partial E_T} \right) \end{bmatrix}$$

where $f_1 = u \xi_x + v \xi_y$ and $f_2 = (E_T + p)/\rho$.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}}_{\nu_1} / \partial \hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial (\hat{\mathbf{E}}_{\nu_1})_4}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{41} \left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{42} \left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{43} \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial E_T} \right) \right]$$

where

$$\left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{41} = -\alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{u^2}{\rho} \right) - \alpha_{yy} \frac{\partial}{\partial \xi} \left(\frac{v^2}{\rho} \right) - 2\alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{uv}{\rho} \right) + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial \rho} \right)$$

$$\left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{42} = \alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) + \alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial(\rho u)} \right)$$

$$\left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{43} = \alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) + \alpha_{yy} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial(\rho v)} \right)$$

$$\alpha_{xx} = (2\mu + \lambda) \xi_x^2 + \mu \xi_y^2$$

$$\alpha_{yy} = \mu \xi_x^2 + (2\mu + \lambda) \xi_y^2$$

$$\alpha_{xy} = (\mu + \lambda) \xi_x \xi_y$$

$$\alpha_0 = \frac{k}{Pr_r} (\xi_x^2 + \xi_y^2)$$

The Jacobian coefficient matrices $\partial \hat{\mathbf{F}}_4 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{F}}_{\nu_1})_4 / \partial \hat{\mathbf{Q}}$ have the same form as $\partial \hat{\mathbf{E}}_4 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{E}}_{\nu_1})_4 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

As an example of how these equations are translated into Fortran, consider the $\Delta(\rho u/J)$ term on the left hand side for the first sweep. This is the second element of $\hat{\mathbf{Q}}$, so using the second element in $\partial \hat{\mathbf{E}}_4 / \partial \hat{\mathbf{Q}}$ we get for the inviscid term

$$A(IV,I,NEN,NRU) = -\frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \left\{ \left(\frac{E_T+p}{\rho} \xi_x \right)_{i-1,j} + \left[(u\xi_x + v\xi_y) \frac{\partial p}{\partial(\rho u)} \right]_{i-1,j} \right\}$$

$$B(IV,I,NEN,NRU) = 0$$

$$C(IV,I,NEN,NRU) = \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \left\{ \left(\frac{E_T+p}{\rho} \xi_x \right)_{i+1,j} + \left[(u\xi_x + v\xi_y) \frac{\partial p}{\partial(\rho u)} \right]_{i+1,j} \right\}$$

For the viscous terms on the left hand side, we use the second element in $\partial(\hat{\mathbf{E}}_{v_1})_4/\partial\hat{\mathbf{Q}}$, which is

$$\frac{1}{Re_r} \left[\alpha_{xx} \frac{\partial}{\partial\xi} \left(\frac{u}{\rho} \right) + \alpha_{xy} \frac{\partial}{\partial\xi} \left(\frac{v}{\rho} \right) + \alpha_0 \frac{\partial}{\partial\xi} \left(\frac{\partial T}{\partial(\rho u)} \right) \right]$$

There are three terms in that element. Thus, in turn, $f = \alpha_{xx}/Re_r$, α_{xy}/Re_r , and α_0/Re_r , and $g = u/\rho$, v/ρ , and $\partial T/\partial(\rho u)$. To add the viscous contribution to this part of the **A** coefficient submatrix, we therefore set

$$A(IV,I,NEN,NRU) = A(IV,I,NEN,NRU) - \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2(\Delta\xi)^2 Re_r} \cdot \left\{ [(\alpha_{xx})_{i-1,j} + (\alpha_{xx})_{i,j}] \left(\frac{u}{\rho} \right)_{i-1,j} + [(\alpha_{xy})_{i-1,j} + (\alpha_{xy})_{i,j}] \left(\frac{v}{\rho} \right)_{i-1,j} + [(\alpha_0)_{i-1,j} + (\alpha_0)_{i,j}] \left(\frac{\partial T}{\partial(\rho u)} \right)_{i-1,j} \right\}$$

Similar equations may be written for the **B** and **C** coefficient submatrices.

The equations for axisymmetric flow are developed in Appendix B of Volume 1. The axisymmetric energy equation for the two ADI sweeps is given by¹⁹

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta(\hat{E}_T)_i + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi^2} \frac{1}{r} \left[\left(r \frac{\partial \hat{E}_s}{\partial \hat{Q}} \right)_{i+1}^n \Delta\hat{Q}_{i+1}^* - \left(r \frac{\partial \hat{E}_s}{\partial \hat{Q}} \right)_{i-1}^n \Delta\hat{Q}_{i-1}^* \right] \\ - \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\xi)^2} \frac{1}{r} \left[(r_{i-1}f_{i-1} + r_i f_i)^n g_{i-1}^n \Delta\hat{Q}_{i-1}^* - (r_{i-1}f_{i-1} + 2r_i f_i + r_{i+1}f_{i+1})^n g_i^n \Delta\hat{Q}_i^* + (r_i f_i + r_{i+1}f_{i+1})^n g_{i+1}^n \Delta\hat{Q}_{i+1}^* \right] = \\ - \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\delta_\xi(r \hat{E}_s) + \delta_\eta(r \hat{F}_s) \right]^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_1})_s] + \delta_\eta[r(\hat{F}_{v_1})_s] \right\}^n \\ + \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_2})_s] + \delta_\eta[r(\hat{F}_{v_2})_s] \right\}^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_2})_s] + \delta_\eta[r(\hat{F}_{v_2})_s] \right\}^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta\hat{E}_T^{n-1} \end{aligned}$$

Sweep 2 (η direction)

$$\begin{aligned} \Delta(\hat{E}_T)_j + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\eta^2} \frac{1}{r} \left[\left(r \frac{\partial \hat{F}_s}{\partial \hat{Q}} \right)_{j+1}^n \Delta\hat{Q}_{j+1}^n - \left(r \frac{\partial \hat{F}_s}{\partial \hat{Q}} \right)_{j-1}^n \Delta\hat{Q}_{j-1}^n \right] \\ - \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\eta)^2} \frac{1}{r} \left[(r_{j-1}f_{j-1} + r_j f_j)^n g_{j-1}^n \Delta\hat{Q}_{j-1}^n - (r_{j-1}f_{j-1} + 2r_j f_j + r_{j+1}f_{j+1})^n g_j^n \Delta\hat{Q}_j^n + (r_j f_j + r_{j+1}f_{j+1})^n g_{j+1}^n \Delta\hat{Q}_{j+1}^n \right] = \\ \Delta\hat{E}_T^* \end{aligned}$$

¹⁹ These equations are written for the general case with swirl. For a non-swirl case, the swirl momentum ρw would not appear as a dependent variable, and the Jacobian coefficient matrices would have only four elements.

where now

$$\begin{aligned}
\hat{\mathbf{Q}} &= \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T \\
\hat{\mathbf{E}}_5 &= \frac{1}{J} [(E_T + p)u\xi_x + (E_T + p)v\xi_r + E_T \xi_t] \\
\hat{\mathbf{F}}_5 &= \frac{1}{J} [(E_T + p)u\eta_x + (E_T + p)v\eta_r + E_T \eta_t] \\
(\hat{\mathbf{E}}_{\nu_1})_5 &= \frac{1}{J} \frac{1}{Re_r} \left\{ \frac{(2\mu + \lambda)}{2} [\xi_x^2(u^2)_\xi + \xi_r^2(v^2)_\xi] + (\mu + \lambda)\xi_x\xi_r(uv)_\xi + \lambda\xi_r \frac{r_\xi}{r} (\xi_r v^2 + \xi_x uv) \right. \\
&\quad \left. + \frac{\mu}{2} [\xi_x^2(v^2 + w^2)_\xi + \xi_r^2(u^2 + w^2)_\xi] + \frac{k}{Pr_r} (\xi_x^2 + \xi_r^2) T_\xi \right\} \\
(\hat{\mathbf{F}}_{\nu_1})_5 &= \frac{1}{J} \frac{1}{Re_r} \left\{ \frac{(2\mu + \lambda)}{2} [\eta_x^2(u^2)_\eta + \eta_r^2(v^2)_\eta] + (\mu + \lambda)\eta_x\eta_r(uv)_\eta + \lambda\eta_r \frac{r_\eta}{r} (\eta_r v^2 + \eta_x uv) \right. \\
&\quad \left. + \frac{\mu}{2} [\eta_x^2(v^2 + w^2)_\eta + \eta_r^2(u^2 + w^2)_\eta] + \frac{k}{Pr_r} (\eta_x^2 + \eta_r^2) T_\eta \right\} \\
(\hat{\mathbf{E}}_{\nu_2})_5 &= \frac{1}{J} \frac{1}{Re_r} \left[2\mu(\xi_x\eta_x uu_\eta + \xi_r\eta_r vv_\eta) + \lambda\xi_x(\eta_x uu_\eta + \eta_r uv_\eta) + \lambda\xi_r(\eta_x vv_\eta + \eta_r vw_\eta) + \lambda\eta_r \frac{v}{r} (\xi_x u + \xi_r v)r_\eta \right. \\
&\quad \left. + \mu\xi_x(\eta_r vv_\eta + \eta_x vw_\eta + \eta_x ww_\eta) + \mu\xi_r(\eta_r uu_\eta + \eta_x uv_\eta + \eta_r ww_\eta) - \mu\xi_r \frac{w^2}{r} \right. \\
&\quad \left. + \frac{k}{Pr_r} (\xi_x\eta_x + \xi_r\eta_r) T_\eta \right] \\
(\hat{\mathbf{F}}_{\nu_2})_5 &= \frac{1}{J} \frac{1}{Re_r} \left[2\mu(\eta_x\xi_x uu_\xi + \eta_r\xi_r vv_\xi) + \lambda\eta_x(\xi_x uu_\xi + \xi_r uv_\xi) + \lambda\eta_r(\xi_x vv_\xi + \xi_r vw_\xi) + \lambda\xi_r \frac{v}{r} (\eta_x u + \eta_r v)r_\xi \right. \\
&\quad \left. + \mu\eta_x(\xi_r vv_\xi + \xi_x vw_\xi + \xi_x ww_\xi) + \mu\eta_r(\xi_r uu_\xi + \xi_x uv_\xi + \xi_r ww_\xi) - \mu\eta_r \frac{w^2}{r} \right. \\
&\quad \left. + \frac{k}{Pr_r} (\eta_x\xi_x + \eta_r\xi_r) T_\xi \right]
\end{aligned}$$

The elements of the Jacobian coefficient matrix $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$ for the inviscid terms in the axisymmetric form of the energy equation are

$$\frac{\partial\hat{\mathbf{E}}_5}{\partial\hat{\mathbf{Q}}} = \begin{bmatrix} -f_1\left(f_2 - \frac{\partial p}{\partial \rho}\right) & f_2\xi_x + f_1\frac{\partial p}{\partial(\rho u)} & f_2\xi_r + f_1\frac{\partial p}{\partial(\rho v)} & f_1\frac{\partial p}{\partial(\rho w)} & \xi_t + f_1\left(1 + \frac{\partial p}{\partial E_T}\right) \end{bmatrix}$$

where $f_1 = u\xi_x + v\xi_r$, and $f_2 = (E_T + p)/\rho$.

The elements of the Jacobian coefficient matrix $\partial\hat{\mathbf{E}}_{\nu_1}/\partial\hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial(\hat{\mathbf{E}}_{\nu_1})_5}{\partial\hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial\hat{\mathbf{E}}_{\nu_1}}{\partial\hat{\mathbf{Q}}} \right)_{s1} \left(\frac{\partial\hat{\mathbf{E}}_{\nu_1}}{\partial\hat{\mathbf{Q}}} \right)_{s2} \left(\frac{\partial\hat{\mathbf{E}}_{\nu_1}}{\partial\hat{\mathbf{Q}}} \right)_{s3} \left(\frac{\partial\hat{\mathbf{E}}_{\nu_1}}{\partial\hat{\mathbf{Q}}} \right)_{s4} \alpha_0 \frac{\partial}{\partial\xi} \left(\frac{\partial T}{\partial E_T} \right) \right]$$

where

$$\begin{aligned}
\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{51} &= -\alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{u^2}{\rho} \right) - \alpha_{rr} \frac{\partial}{\partial \xi} \left(\frac{v^2}{\rho} \right) - \alpha_{zz} \frac{\partial}{\partial \xi} \left(\frac{w^2}{\rho} \right) \\
&\quad - 2\alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{uv}{\rho} \right) - 2\alpha'_{rr} \frac{v^2}{\rho} r_\xi - 2\alpha'_{xr} \frac{uv}{\rho} r_\xi + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial \rho} \right) \\
\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{52} &= \alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) + \alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) + \alpha'_{xr} \frac{v}{\rho} r_\xi + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial(\rho u)} \right) \\
\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{53} &= \alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) + \alpha_{rr} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) + \alpha'_{rr} \frac{v}{\rho} r_\xi + \alpha'_{xr} \frac{v}{\rho} r_\xi + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial(\rho v)} \right) \\
\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{54} &= \alpha_{zz} \frac{\partial}{\partial \xi} \left(\frac{w}{\rho} \right) + \alpha_0 \frac{\partial}{\partial \xi} \left(\frac{\partial T}{\partial(\rho w)} \right) \\
\alpha_{xx} &= (2\mu + \lambda) \xi_x^2 + \mu \xi_r^2 \\
\alpha_{rr} &= \mu \xi_x^2 + (2\mu + \lambda) \xi_r^2 \\
\alpha_{zz} &= \mu \xi_x^2 + \mu \xi_r^2 \\
\alpha_{xr} &= (\mu + \lambda) \xi_x \xi_r \\
\alpha'_{xr} &= \frac{\lambda}{r} \xi_x \xi_r \\
\alpha'_{rr} &= \frac{\lambda}{r} \xi_r^2 \\
\alpha_0 &= \frac{k}{Pr_r} (\xi_x^2 + \xi_r^2)
\end{aligned}$$

As in 2-D planar flow, the Jacobian coefficient matrices $\partial \hat{\mathbf{F}}_s / \partial \hat{\mathbf{Q}}$ and $\partial(\hat{\mathbf{F}}_{V_1})_s / \partial \hat{\mathbf{Q}}$ have the same form as $\partial \hat{\mathbf{E}}_s / \partial \hat{\mathbf{Q}}$ and $\partial(\hat{\mathbf{E}}_{V_1})_s / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

Note that the equations for 2-D planar and axisymmetric flow are very similar. In the axisymmetric equations there are some additional terms involving the radius r in the viscous flux vectors, with corresponding terms in the Jacobian coefficient matrices. The radius r appears as an additional coefficient in front of the flux vectors $\hat{\mathbf{E}}$, $\hat{\mathbf{E}}_{V_1}$, etc., and in front of the Jacobian coefficient matrices $\partial \hat{\mathbf{E}}_s / \partial \hat{\mathbf{Q}}$, $\partial(\hat{\mathbf{E}}_{V_1})_s / \partial \hat{\mathbf{Q}}$, etc. In addition, $1/r$ appears in front of every term in the equation except the $\Delta \hat{E}_T$ terms. In *Proteus*, the Fortran variables are defined in such a way that, for many terms, the same coding can be used for both 2-D planar and axisymmetric flow. Unfortunately, this may make some of the coding a little confusing. It is hoped that this detailed description, when compared with the source listing, will help make things clear.

In COEFE, the coefficients of the left hand side, or implicit, terms are defined first. The implicit terms for the second ADI sweep have exactly the same form as for the first sweep, but with ξ replaced by η . By defining DEL, METX, METY, and METT as the grid spacing and metric coefficients in the sweep direction, the same coding can be used for both sweeps. The variable RAX is equal to 1 for 2-D planar flow, and the radius r for axisymmetric flow. This adds the r in front of the Jacobian coefficient matrices for axisymmetric flow, but has no effect for 2-D planar flow. The $1/r$ coefficient in front of each term will be

added later. In this section of code, the coefficient of $\Delta \hat{E}_T$ (part of $B(IV,I,NEN,NET)$) is set equal to r , not 1 as it should be. This will be corrected later.

The source term, or right hand side, for the first sweep is defined next. The difference formulas used to compute the source term are the same as those used for the implicit terms. These formulas are presented in Section 5.0 of Volume 1. For axisymmetric flow, the Fortran variable $J1$, which is normally defined as $1/J$, is temporarily redefined as r/J before the COEF routines are called. This automatically accounts for the r coefficient in front of all the flux vectors in the source term. The $1/r$ coefficient in front of each term will be added later. This definition of $J1$ adds an r in front of the $\Delta \hat{E}_T^{-1}$ term that should not be there. This will also be corrected later.

The coding for the source term for the second sweep, which consists only of $\Delta \hat{E}_T^*$, comes next. The definition of $J1$ also adds an r in front of this term that should not be there.

And finally, for axisymmetric flow, the entire equation is divided by the local radius r . This adds the $1/r$ coefficient where it should be added, and removes the r in front of the $\Delta \hat{E}_T$ terms.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For sections of the code that apply to both sweeps (i.e., the implicit terms and the division by r at the end), the first two subscripts are written as (IV,I). For sections of the code that apply only to the first sweep, the first two subscripts are written as (I2,I1). For sections that apply only to the second sweep, they are written as (I1,I2). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.
3. The coding of the extra coefficients and source terms in the axisymmetric form of the equations is separate from the rest of the coding, and is bypassed if the flow is not axisymmetric. Similarly, the coding of coefficients and source terms involving the swirl velocity is separate from the rest of the coding, and is bypassed if there is no swirl.
4. The Euler option is implemented simply by skipping the calculation of the coefficients and source terms for the viscous and heat conduction terms.
5. The thin-layer option is implemented by skipping the calculation of the coefficients and source terms for the viscous and heat conduction terms containing derivatives in the specified direction.

Subroutine COEFS1 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXECT		Compute coefficients and source terms for the k and ε equations for the first ADI sweep.

Input

* CMUR	Constant C_{μ} in formula for C_{μ} .
* CTHREE	Constant C_3 in formula for C_{μ} .
* CTWOR	Constant C_2 in formula for C_2 .
DTAU	Time step $\Delta\tau$.
DUMMY	Distance to the nearest solid wall.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
E, EL	Turbulent dissipation rate ε at time levels n and $n - 1$.
ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric).
* IAXI	Flag for axisymmetric flow.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KE, KEL	Turbulent kinetic energy k at time levels n and $n - 1$.
MU	Laminar viscosity μ_l at time level n .
MUT, MUTL	Turbulent viscosity μ_t at time levels n and $n - 1$.
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
* RER	Reference Reynolds number Re_r .
RHO, U, V	Static density ρ , and velocities u and v , at time level n .
RHOL	Static density ρ at time level $n - 1$.
* SIGE, SIGK	Constants σ_ε and σ_k used in the diffusion term of the ε equation.
* TFACT	Factor used in computing the k - ε time step.
* THKE	Parameters θ_1 and θ_2 determining type of time differencing for the k - ε equations.
VORT	Production rate of turbulent kinetic energy.
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ_r if axisymmetric).
Y	Radial coordinate r for axisymmetric flow.
YPLUSD	Nondimensional distance y^+ from the nearest solid wall.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points.
S	Source term subvector S at interior points.

Description

Subroutine COEFS1 computes the coefficients and source terms for the k - ε equations for the first ADI sweep. Equation (9.40a) in Volume 1 represents, in vector form, the governing equation for the first ADI sweep for 2-D planar flow. This equation may be written in difference form as:

$$\begin{aligned} & \begin{bmatrix} 1 - T_1 Z_{11} & -T_1 Z_{12} \\ -T_1 Z_{21} & 1 - T_1 Z_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} + T_1 \left\{ (\delta_u)_\xi \left(\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) - \delta_\xi \left(\begin{bmatrix} B_{11} & 0 \\ 0 & B_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) \right\} = \\ & T_1 (\delta_\xi \hat{\mathbf{F}}_M^n - \delta_\xi \hat{\mathbf{F}}_M^{n-1} + \delta_\eta \hat{\mathbf{G}}_M^n - \delta_\eta \hat{\mathbf{G}}_M^{n-1}) \\ & + T_2 \left(-(\delta_u)_\xi \hat{\mathbf{F}}_C^n + \delta_\xi \hat{\mathbf{F}}_D^n + \delta_\xi \hat{\mathbf{F}}_M^n - (\delta_u)_\eta \hat{\mathbf{G}}_C^n + \delta_\eta \hat{\mathbf{G}}_D^n + \delta_\eta \hat{\mathbf{G}}_M^n + \hat{\mathbf{S}}^n + \hat{\mathbf{T}}^n \right) + T_3 \Delta \hat{\mathbf{W}}^{n-1} \end{aligned}$$

where

$$T_1 = \frac{\theta_1 \Delta \tau}{1 + \theta_2}$$

$$T_2 = \frac{\Delta \tau}{1 + \theta_2}$$

$$T_3 = \frac{\theta_2}{1 + \theta_2}$$

In the above equation, Z_{11} , etc., are elements of a matrix Z , defined as $Z = M + N$, and A , B , M , and N are the Jacobian coefficient matrices defined in equations (9.31), (9.32), (9.35), and (9.36) of Volume 1. Also, $(\delta_u)_\xi$ is the first-order upwind difference operator used for the convective terms, and δ_ξ is the second-order central difference operator used for the viscous terms.

The convective term on the left side can thus be expanded as:

$$(\delta_u)_\xi \left(\begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) = \begin{cases} \frac{1}{\Delta \xi} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_i - \frac{1}{\Delta \xi} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_{i-1} & \text{if } \xi_x u + \xi_y v > 0 \\ \frac{1}{\Delta \xi} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_{i+1} - \frac{1}{\Delta \xi} \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_i & \text{if } \xi_x u + \xi_y v < 0 \end{cases}$$

In the above equations, and in those to follow, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j .

The Jacobian coefficient matrix B may be written as:

$$B = \begin{bmatrix} f g_{\xi(11)} & 0 \\ 0 & f g_{\xi(22)} \end{bmatrix}$$

The viscous term on the left hand side may thus be expanded as:

$$\delta_{\xi} \left(\begin{bmatrix} B_{11} & 0 \\ 0 & B_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) = \frac{1}{2(\Delta \xi)^2} \left(\begin{aligned} & \begin{bmatrix} (f_{i-1} + f_i)g_{i-1(11)} & 0 \\ 0 & (f_{i-1} + f_i)g_{i-1(22)} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_{i-1} \\ & - \begin{bmatrix} (f_{i+1} + 2f_i + f_{i-1})g_{i(11)} & 0 \\ 0 & (f_{i+1} + 2f_i + f_{i-1})g_{i(22)} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_i \\ & + \begin{bmatrix} (f_i + f_{i+1})g_{i+1(11)} & 0 \\ 0 & (f_i + f_{i+1})g_{i+1(22)} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}_{i+1} \end{aligned} \right)$$

On the right hand side, the convective term $(\delta_u)_\xi \hat{\mathbf{F}}_C$ is differenced as:

$$(\delta_u)_\xi \hat{\mathbf{F}}_C = \begin{cases} \frac{1}{\Delta \xi} [(\hat{\mathbf{F}}_C)_i - (\hat{\mathbf{F}}_C)_{i-1}] & \text{if } \xi_x u + \xi_y v > 0 \\ \frac{1}{\Delta \xi} [(\hat{\mathbf{F}}_C)_{i+1} - (\hat{\mathbf{F}}_C)_i] & \text{if } \xi_x u + \xi_y v < 0 \end{cases}$$

An analogous expression may be written for $(\delta_u)_\eta \hat{\mathbf{G}}_C$. The vectors $\hat{\mathbf{F}}_D$ and $\hat{\mathbf{F}}_M$ may be written as

$$\hat{\mathbf{F}}_D = \begin{bmatrix} f g_{\xi(1)} \\ f g_{\xi(2)} \end{bmatrix}$$

$$\hat{\mathbf{F}}_M = \begin{bmatrix} f g_{\eta(1)} \\ f g_{\eta(2)} \end{bmatrix}$$

The terms $\delta_\xi \hat{\mathbf{F}}_D$ and $\delta_\xi \hat{\mathbf{F}}_M$ are thus differenced as:

$$\delta_\xi \hat{\mathbf{F}}_D = \frac{1}{2(\Delta \xi)^2} \left\{ \begin{aligned} & \begin{bmatrix} (f_{i-1} + f_i)g_{i-1(1)} \\ (f_{i-1} + f_i)g_{i-1(2)} \end{bmatrix} - \begin{bmatrix} (f_{i+1} + 2f_i + f_{i-1})g_{i(1)} \\ (f_{i+1} + 2f_i + f_{i-1})g_{i(2)} \end{bmatrix} + \begin{bmatrix} (f_i + f_{i+1})g_{i+1(1)} \\ (f_i + f_{i+1})g_{i+1(2)} \end{bmatrix} \end{aligned} \right\}$$

$$\delta_\xi \hat{\mathbf{F}}_M = \frac{1}{4\Delta \xi \Delta \eta} \left\{ \begin{aligned} & \begin{bmatrix} f_{i+1,j}(g_{i+1,j+1} - g_{i+1,j-1})_{(1)} \\ f_{i+1,j}(g_{i+1,j+1} - g_{i+1,j-1})_{(2)} \end{bmatrix} - \begin{bmatrix} f_{i-1,j}(g_{i-1,j+1} - g_{i-1,j-1})_{(1)} \\ f_{i-1,j}(g_{i-1,j+1} - g_{i-1,j-1})_{(2)} \end{bmatrix} \end{aligned} \right\}$$

Analogous expressions may be written for $\delta_\eta \hat{\mathbf{G}}_D$ and $\delta_\eta \hat{\mathbf{G}}_M$.

The k - ε equations for axisymmetric flow are presented in Appendix B of Volume 1. They may be written in difference form for the first ADI sweep as:

$$\begin{aligned} & \left[\begin{bmatrix} 1 - T_1 Z_{11} & -T_1 Z_{12} \\ -T_1 Z_{21} & 1 - T_1 Z_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} + \frac{T_1}{r} \left\{ (\delta_u)_\xi \left(r \begin{bmatrix} A_{11} & 0 \\ 0 & A_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) - \delta_\xi \left(r \begin{bmatrix} B_{11} & 0 \\ 0 & B_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix} \right) \right\} = \\ & \frac{T_1}{r} (\delta_\xi r \hat{\mathbf{F}}_M^n - \delta_\xi r \hat{\mathbf{F}}_M^{n-1} + \delta_\eta r \hat{\mathbf{G}}_M^n - \delta_\eta r \hat{\mathbf{G}}_M^{n-1}) \\ & + \frac{T_2}{r} \left(-(\delta_u)_\xi r \hat{\mathbf{F}}_C^n + \delta_\xi r \hat{\mathbf{F}}_D^n + \delta_\xi r \hat{\mathbf{F}}_M^n - (\delta_u)_\eta r \hat{\mathbf{G}}_C^n + \delta_\eta r \hat{\mathbf{G}}_D^n + \delta_\eta r \hat{\mathbf{G}}_M^n + r \hat{\mathbf{S}}^n + r \hat{\mathbf{T}}^n \right) + T_3 \Delta \hat{\mathbf{W}}^{n-1} \end{aligned}$$

where r is the radial coordinate and all other terms are the same as the 2-D planar equations presented above.

Remarks

1. For the variables A, B, C, and S, the first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. Since this subroutine only applies to the first sweep, the first two subscripts of A, B, C, and S variables are written as (J,I). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.
2. For axisymmetric flows, the Fortran variables RIJ, RIP1J, and RIM1J are the cylindrical r coordinates for the grid points (I,J), (I + 1,J), and (I - 1,J), respectively. Similarly, RIJP1 and RIJM1 are the cylindrical r coordinates for the grid points (I,J + 1) and (I,J - 1). For 2-D flows, all of these variables are set equal to 1.0.

Subroutine COEFS2 (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXECT		Compute coefficients and source terms for the k and ε equations for the second ADI sweep.

Input

DETA	Computational grid spacing $\Delta\eta$.
DTAU	Time step $\Delta\tau$.
E, EL	Turbulent dissipation rate ε at time levels n and $n - 1$.
ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric).
* IAXI	Flag for axisymmetric flow.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KE, KEL	Turbulent kinetic energy k at time levels n and $n - 1$.
MU	Laminar viscosity μ_l at time level n .
MUT	Turbulent viscosity μ_t at time level n .
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
* RER	Reference Reynolds number Re_r .
RHO, U, V	Static density ρ , and velocities u and v , at time level n .
RHOL	Static density ρ at time level $n - 1$.
S	Computed solution subvector from first sweep.
* SIGE, SIGK	Constants σ_ε and σ_k used in the diffusion term of the ε equation.
* TFACT	Factor used in computing the k - ε time step.
* THKE	Parameters θ_1 and θ_2 determining type of time differencing for the k - ε equations.
Y	Radial coordinate r for axisymmetric flow.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points.
S	Source term subvector S at interior points.

Description

Subroutine COEFS2 computes the coefficients and source terms for the k - ε equations for the second ADI sweep. Equation (9.40b) in Volume 1 represents, in vector form, the governing equation for the second ADI sweep for 2-D planar flow. This equation may be written in difference form as:

$$\begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} + T_1 \left\{ (\delta_u)_\eta \left(\begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) - \delta_\eta \left(\begin{bmatrix} D_{11} & 0 \\ 0 & D_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) \right\} = \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}$$

where

$$T_1 = \frac{\theta_1 \Delta \tau}{1 + \theta_2}$$

In the above equation C and D are the Jacobian coefficient matrices defined in equations (9.33) and (9.34) of Volume 1. Also, $(\delta_u)_\eta$ is the first-order upwind difference operator used for the convective terms, and δ_η is the second-order central difference operator used for the viscous terms.

The convective term on the left side can thus be expanded as:

$$(\delta_u)_\eta \left(\begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) = \begin{cases} \frac{1}{\Delta \eta} \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j-1} - \frac{1}{\Delta \eta} \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j+1} & \text{if } \eta_x u + \eta_y v > 0 \\ \frac{1}{\Delta \eta} \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j+1} - \frac{1}{\Delta \eta} \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j-1} & \text{if } \eta_x u + \eta_y v < 0 \end{cases}$$

In the above equations, and in those to follow, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j .

The Jacobian coefficient matrix D may be written as:

$$D = \begin{bmatrix} f g_{\eta(11)} & 0 \\ 0 & f g_{\eta(22)} \end{bmatrix}$$

The viscous term on the left hand side may thus be expanded as:

$$\delta_\eta \left(\begin{bmatrix} D_{11} & 0 \\ 0 & D_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) = \frac{1}{2(\Delta \xi)^2} \left(\begin{bmatrix} (f_{j-1} + f_j) g_{j-1}(11) & 0 \\ 0 & (f_{j-1} + f_j) g_{j-1}(22) \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j-1} \right. \\ \left. - \begin{bmatrix} (f_{j+1} + 2f_j + f_{j-1}) g_j(11) & 0 \\ 0 & (f_{j+1} + 2f_j + f_{j-1}) g_j(22) \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_j \right. \\ \left. + \begin{bmatrix} (f_j + f_{j+1}) g_{j+1}(11) & 0 \\ 0 & (f_j + f_{j+1}) g_{j+1}(22) \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix}_{j+1} \right)$$

The k - ε equations for axisymmetric flow are presented in Appendix B of Volume 1. They may be written in difference form for the second ADI sweep as:

$$\begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} + \frac{T_1}{r} \left\{ (\delta_u)_\eta \left(r \begin{bmatrix} C_{11} & 0 \\ 0 & C_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) - \delta_\eta \left(r \begin{bmatrix} D_{11} & 0 \\ 0 & D_{22} \end{bmatrix} \begin{bmatrix} \Delta \hat{W}_1^n \\ \Delta \hat{W}_2^n \end{bmatrix} \right) \right\} = \begin{bmatrix} \Delta \hat{W}_1^* \\ \Delta \hat{W}_2^* \end{bmatrix}$$

where r is the radial coordinate and all other terms are the same as the 2-D planar equations presented above.

Remarks

1. For the variables A, B, C, and S, the first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. Since this subroutine only ap-

plies to the second sweep, the first two subscripts of A, B, C, and S variables are written as (I,J). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.

2. For axisymmetric flows, the Fortran variables RIJ, RIJP1, and RIJM1 are the cylindrical r coordinates for the grid points (I,J), (I,J + 1), and (I,J - 1), respectively. For 2-D flows, these variables are set equal to 1.0.

Subroutine COEFX (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Compute coefficients and source term for the x-momentum equation.

Input

DEL	Computational grid spacing in sweep direction.
DPDRHO, DPDRU, DPDRV, DPDRW, DPDET	Derivatives $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, $\partial p/\partial(\rho v)$, $\partial p/\partial(\rho w)$, and $\partial p/\partial E_T$.
DTAU	Time step $\Delta \tau$.
DXI, DETA	Computational grid spacing $\Delta \xi$ and $\Delta \eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* IAXI	Flag for axisymmetric flow.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IEULER	Flag for Euler calculation.
* IHSTAG	Flag for constant stagnation enthalpy option.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
* ITHIN	Flags for thin-layer option.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} (times the radius r for axisymmetric flow.)
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
MU, LA	Effective coefficient of viscosity μ and effective second coefficient of viscosity λ at time level n .
NEQ	Number of coupled equations being solved, N_{eq} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, METY, and METT.
NXM	Array index associated with the x-momentum equation.
P	Static pressure p at time level n .
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow.
* RER	Reference Reynolds number Re_r .
RHO, U, V	Static density ρ , and velocities u and v at time level n .
RHOL, UL, VL	Static density ρ , and velocities u and v from previous ADI sweep.

* THX	Parameters θ_1 , θ_2 , and θ_3 determining type of time differencing for the x-momentum equation.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .
Y	Radial coordinate r for axisymmetric flow.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points (row NXM only).
S	Source term subvector S at interior points (element NXM only).

Description

Subroutine COEFX computes the coefficients and source term for the x-momentum equation. Equations (7.5a-b) in Volume 1 represent, in vector form, the four governing difference equations for the two ADI sweeps for 2-D planar flow. The elements of the inviscid flux vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{F}}$ are given in Section 2.0 of Volume 1, and the elements of the viscous flux vectors $\hat{\mathbf{E}}_{\nu_1}$, $\hat{\mathbf{E}}_{\nu_2}$, etc., are given in Appendix A of Volume 1. The Jacobian coefficient matrices $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$, $\partial\hat{\mathbf{E}}_{\nu_1}/\partial\hat{\mathbf{Q}}$, etc., are given in Section 4.0 of Volume 1. Using all of these equations, the differenced form of the x-momentum equation for 2-D planar flow may be written for the two ADI sweeps as²⁰

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta(\hat{\rho}u)_i^* + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \xi} \left[\left(\frac{\partial \hat{\mathbf{E}}_2}{\partial \hat{\mathbf{Q}}} \right)_{i+1}^n \Delta \hat{\mathbf{Q}}_{i+1}^* - \left(\frac{\partial \hat{\mathbf{E}}_2}{\partial \hat{\mathbf{Q}}} \right)_{i-1}^n \Delta \hat{\mathbf{Q}}_{i-1}^* \right] \\ - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \xi)^2} \left[(f_{i-1} + f_i)^n g_{i-1}^n \Delta \hat{\mathbf{Q}}_{i-1}^* - (f_{i-1} + 2f_i + f_{i+1})^n g_i^n \Delta \hat{\mathbf{Q}}_i^* + (f_i + f_{i+1})^n g_{i+1}^n \Delta \hat{\mathbf{Q}}_{i+1}^* \right] = \\ - \frac{\Delta \tau}{1 + \theta_2} (\delta_\xi \hat{\mathbf{E}}_2 + \delta_\eta \hat{\mathbf{F}}_2)^n + \frac{\Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_1})_2 + \delta_\eta (\hat{\mathbf{F}}_{\nu_1})_2]^n \\ + \frac{(1 + \theta_3) \Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_2})_2 + \delta_\eta (\hat{\mathbf{F}}_{\nu_2})_2]^n - \frac{\theta_3 \Delta \tau}{1 + \theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_2})_2 + \delta_\eta (\hat{\mathbf{F}}_{\nu_2})_2]^{n-1} + \frac{\theta_2}{1 + \theta_2} \Delta(\hat{\rho}u)^{n-1} \end{aligned}$$

Sweep 2 (η direction)

$$\begin{aligned} \Delta(\hat{\rho}u)_j^n + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \eta} \left[\left(\frac{\partial \hat{\mathbf{F}}_2}{\partial \hat{\mathbf{Q}}} \right)_{j+1}^n \Delta \hat{\mathbf{Q}}_{j+1}^n - \left(\frac{\partial \hat{\mathbf{F}}_2}{\partial \hat{\mathbf{Q}}} \right)_{j-1}^n \Delta \hat{\mathbf{Q}}_{j-1}^n \right] \\ - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \eta)^2} \left[(f_{j-1} + f_j)^n g_{j-1}^n \Delta \hat{\mathbf{Q}}_{j-1}^n - (f_{j-1} + 2f_j + f_{j+1})^n g_j^n \Delta \hat{\mathbf{Q}}_j^n + (f_j + f_{j+1})^n g_{j+1}^n \Delta \hat{\mathbf{Q}}_{j+1}^n \right] = \\ \Delta(\hat{\rho}u)^* \end{aligned}$$

²⁰ These equations are written assuming the energy equation is being solved. For a constant stagnation enthalpy case, the total energy E_T would not appear as a dependent variable, and the Jacobian coefficient matrices would have only three elements.

In the above equations, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j . On the left hand side, f is the coefficient of $\partial/\partial\xi$ (or $\partial/\partial\eta$, depending on the sweep) in the $\partial\hat{\mathbf{E}}_{v_1}/\partial\hat{\mathbf{Q}}$ (or $\partial\hat{\mathbf{F}}_{v_1}/\partial\hat{\mathbf{Q}}$) Jacobian coefficient matrix. Similarly, g is the term in the parentheses following $\partial/\partial\xi$ (or $\partial/\partial\eta$) in the $\partial\hat{\mathbf{E}}_{v_1}/\partial\hat{\mathbf{Q}}$ (or $\partial\hat{\mathbf{F}}_{v_1}/\partial\hat{\mathbf{Q}}$) Jacobian coefficient matrix.

The vector of dependent variables is

$$\hat{\mathbf{Q}} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad E_T]^T$$

The appropriate elements of the inviscid flux vectors are given by

$$\hat{\mathbf{E}}_2 = \frac{1}{J} [(\rho u^2 + p)\xi_x + \rho uv\xi_y + \rho u\xi_t]$$

$$\hat{\mathbf{F}}_2 = \frac{1}{J} [(\rho u^2 + p)\eta_x + \rho uv\eta_y + \rho u\eta_t]$$

The appropriate elements of the non-cross derivative viscous flux vectors are

$$(\hat{\mathbf{E}}_{v_1})_2 = \frac{1}{J} \frac{1}{Re_r} [2\mu\xi_x^2 u_\xi + \lambda\xi_x(\xi_x u_\xi + \xi_y v_\xi) + \mu\xi_y(\xi_y u_\xi + \xi_x v_\xi)]$$

$$(\hat{\mathbf{F}}_{v_1})_2 = \frac{1}{J} \frac{1}{Re_r} [2\mu\eta_x^2 u_\eta + \lambda\eta_x(\eta_x u_\eta + \eta_y v_\eta) + \mu\eta_y(\eta_y u_\eta + \eta_x v_\eta)]$$

And the appropriate elements of the cross derivative viscous flux vectors are

$$(\hat{\mathbf{E}}_{v_2})_2 = \frac{1}{J} \frac{1}{Re_r} [2\mu\xi_x\eta_x u_\eta + \lambda\xi_x(\eta_x u_\eta + \eta_y v_\eta) + \mu\xi_y(\eta_y u_\eta + \eta_x v_\eta)]$$

$$(\hat{\mathbf{F}}_{v_2})_2 = \frac{1}{J} \frac{1}{Re_r} [2\mu\eta_x\xi_x u_\xi + \lambda\eta_x(\xi_x u_\xi + \xi_y v_\xi) + \mu\eta_y(\xi_y u_\xi + \xi_x v_\xi)]$$

The elements of the Jacobian coefficient matrix $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$ for the inviscid terms in the x-momentum equation are

$$\frac{\partial\hat{\mathbf{E}}_2}{\partial\hat{\mathbf{Q}}} = \begin{bmatrix} \frac{\partial p}{\partial\rho} \xi_x - uf_1 & \xi_t + f_1 + u\xi_x + \frac{\partial p}{\partial(\rho u)} \xi_x & u\xi_y + \frac{\partial p}{\partial(\rho v)} \xi_x & \frac{\partial p}{\partial E_T} \xi_x \end{bmatrix}$$

where $f_1 = u\xi_x + v\xi_y$.

The elements of the Jacobian coefficient matrix $\partial\hat{\mathbf{E}}_{v_1}/\partial\hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial(\hat{\mathbf{E}}_{v_1})_2}{\partial\hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial\hat{\mathbf{E}}_{v_1}}{\partial\hat{\mathbf{Q}}} \right)_{21} \alpha_{xx} \frac{\partial}{\partial\xi} \left(\frac{1}{\rho} \right) \alpha_{xy} \frac{\partial}{\partial\xi} \left(\frac{1}{\rho} \right) \quad 0 \right]$$

where

$$\left(\frac{\partial\hat{\mathbf{E}}_{v_1}}{\partial\hat{\mathbf{Q}}} \right)_{21} = -\alpha_{xx} \frac{\partial}{\partial\xi} \left(\frac{u}{\rho} \right) - \alpha_{xy} \frac{\partial}{\partial\xi} \left(\frac{v}{\rho} \right)$$

$$\alpha_{xx} = (2\mu + \lambda)\xi_x^2 + \mu\xi_y^2$$

$$\alpha_{xy} = (\mu + \lambda)\xi_x\xi_y$$

The Jacobian coefficient matrices $\partial\hat{\mathbf{F}}_2/\partial\hat{\mathbf{Q}}$ and $\partial(\hat{\mathbf{F}}_{v1})_2/\partial\hat{\mathbf{Q}}$ have the same form as $\partial\hat{\mathbf{E}}_2/\partial\hat{\mathbf{Q}}$ and $\partial(\hat{\mathbf{E}}_{v1})_2/\partial\hat{\mathbf{Q}}$, but with ξ replaced by η .

As an example of how these equations are translated into Fortran, consider the $\Delta(\rho u/J)$ term on the left hand side for the first sweep. This is the second element of $\hat{\mathbf{Q}}$, so using the second element in $\partial\hat{\mathbf{E}}_2/\partial\hat{\mathbf{Q}}$, and including the $\Delta(\rho u)_i^*$ term, we get for the inviscid term

$$A(\text{IV},\text{I},\text{NXM},\text{NRU}) = -\frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \left[(\xi_t)_{i-1,j} + (u\xi_x + v\xi_y)_{i-1,j} + (u\xi_x)_{i-1,j} + \left(\frac{\partial p}{\partial(\rho u)} \xi_x \right)_{i-1,j} \right]$$

$$B(\text{IV},\text{I},\text{NXM},\text{NRU}) = 1$$

$$C(\text{IV},\text{I},\text{NXM},\text{NRU}) = \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \left[(\xi_t)_{i+1,j} + (u\xi_x + v\xi_y)_{i+1,j} + (u\xi_x)_{i+1,j} + \left(\frac{\partial p}{\partial(\rho u)} \xi_x \right)_{i+1,j} \right]$$

For the viscous terms on the left hand side, we use the second element in $\partial(\hat{\mathbf{E}}_{v1})_2/\partial\hat{\mathbf{Q}}$, which is

$$\frac{1}{Re_r} \alpha_{xx} \frac{\partial}{\partial\xi} \left(\frac{1}{\rho} \right)$$

Thus $f = \alpha_{xx}/Re_r$ and $g = 1/\rho$. To add the viscous contribution to this part of the A coefficient submatrix, we therefore set

$$A(\text{IV},\text{I},\text{NXM},\text{NRU}) = A(\text{IV},\text{I},\text{NXM},\text{NRU}) - \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2(\Delta\xi)^2 Re_r} [(\alpha_{xx})_{i-1,j} + (\alpha_{xx})_{i,j}] \left(\frac{1}{\rho} \right)_{i-1,j}$$

Similar equations may be written for the B and C coefficient submatrices.

The equations for axisymmetric flow are developed in Appendix B of Volume 1. The axisymmetric x-momentum equation for the two ADI sweeps is given by²¹

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta(\rho u)_i^* + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi} \frac{1}{r} \left[\left(r \frac{\partial\hat{\mathbf{E}}_2}{\partial\hat{\mathbf{Q}}} \right)_{i+1}^n \Delta\hat{\mathbf{Q}}_{i+1}^* - \left(r \frac{\partial\hat{\mathbf{E}}_2}{\partial\hat{\mathbf{Q}}} \right)_{i-1}^n \Delta\hat{\mathbf{Q}}_{i-1}^* \right] \\ - \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\xi)^2} \frac{1}{r} \left[(r_{i-1}f_{i-1} + r_i f_i) g_{i-1}^n \Delta\hat{\mathbf{Q}}_{i-1}^* - (r_{i-1}f_{i-1} + 2r_i f_i + r_{i+1}f_{i+1}) g_i^n \Delta\hat{\mathbf{Q}}_i^* + (r_i f_i + r_{i+1}f_{i+1}) g_{i+1}^n \Delta\hat{\mathbf{Q}}_{i+1}^* \right] = \\ - \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\delta_\xi(r\hat{\mathbf{E}}_2) + \delta_\eta(r\hat{\mathbf{F}}_2) \right]^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{\mathbf{E}}_{v1})_2] + \delta_\eta[r(\hat{\mathbf{F}}_{v1})_2] \right\}^n \\ + \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{\mathbf{E}}_{v2})_2] + \delta_\eta[r(\hat{\mathbf{F}}_{v2})_2] \right\}^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{\mathbf{E}}_{v2})_2] + \delta_\eta[r(\hat{\mathbf{F}}_{v2})_2] \right\}^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta(\rho u)^{n-1} \end{aligned}$$

²¹ These equations are written for the general case with swirl. For a non-swirl case, the swirl momentum ρw would not appear as a dependent variable, and the Jacobian coefficient matrices would have only four elements.

Sweep 2 (η direction)

$$\Delta(\hat{\rho}u)_j^n + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \eta} \frac{1}{r} \left[\left(r \frac{\partial \hat{\mathbf{F}}_2}{\partial \hat{\mathbf{Q}}} \right)_{j+1}^n \Delta \hat{\mathbf{Q}}_{j+1}^n - \left(r \frac{\partial \hat{\mathbf{F}}_2}{\partial \hat{\mathbf{Q}}} \right)_{j-1}^n \Delta \hat{\mathbf{Q}}_{j-1}^n \right] \\ - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \eta)^2} \frac{1}{r} \left[(r_{j-1} f_{j-1} + r_j f_j) g_{j-1}^n \Delta \hat{\mathbf{Q}}_{j-1}^n - (r_{j-1} f_{j-1} + 2r_j f_j + r_{j+1} f_{j+1}) g_j^n \Delta \hat{\mathbf{Q}}_j^n + (r_j f_j + r_{j+1} f_{j+1}) g_{j+1}^n \Delta \hat{\mathbf{Q}}_{j+1}^n \right] = \\ \Delta(\hat{\rho}u)_j^n$$

where now

$$\hat{\mathbf{Q}} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T$$

$$\hat{\mathbf{E}}_2 = \frac{1}{J} [(\rho u^2 + p) \xi_x + \rho u v \xi_r + \rho u \xi_t]$$

$$\hat{\mathbf{F}}_2 = \frac{1}{J} [(\rho u^2 + p) \eta_x + \rho u v \eta_r + \rho u \eta_t]$$

$$(\hat{\mathbf{E}}_{\nu_1})_2 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \xi_x^2 u_\xi + \lambda \xi_x \left[\xi_x u_\xi + \frac{1}{r} \xi_r (rv)_\xi \right] + \mu \xi_r (\xi_r u_\xi + \xi_x v_\xi) \right\}$$

$$(\hat{\mathbf{F}}_{\nu_1})_2 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \eta_x^2 u_\eta + \lambda \eta_x \left[\eta_x u_\eta + \frac{1}{r} \eta_r (rv)_\eta \right] + \mu \eta_r (\eta_r u_\eta + \eta_x v_\eta) \right\}$$

$$(\hat{\mathbf{E}}_{\nu_2})_2 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \xi_x \eta_x u_\eta + \lambda \xi_x \left[\eta_x u_\eta + \frac{1}{r} \eta_r (rv)_\eta \right] + \mu \xi_r (\eta_r u_\eta + \eta_x v_\eta) \right\}$$

$$(\hat{\mathbf{F}}_{\nu_2})_2 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \eta_x \xi_x u_\xi + \lambda \eta_x \left[\xi_x u_\xi + \frac{1}{r} \xi_r (rv)_\xi \right] + \mu \eta_r (\xi_r u_\xi + \xi_x v_\xi) \right\}$$

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}} / \partial \hat{\mathbf{Q}}$ for the inviscid terms in the axisymmetric form of the energy equation are

$$\frac{\partial \hat{\mathbf{E}}_2}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} \frac{\partial p}{\partial \rho} \xi_x - u f_1 & \xi_t + f_1 + u \xi_x + \frac{\partial p}{\partial (\rho u)} \xi_x & u \xi_r + \frac{\partial p}{\partial (\rho v)} \xi_x & \frac{\partial p}{\partial (\rho w)} \xi_x & \frac{\partial p}{\partial E_T} \xi_x \end{bmatrix}$$

where $f_1 = u \xi_x + v \xi_r$.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}}_{\nu_1} / \partial \hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial (\hat{\mathbf{E}}_{\nu_1})_2}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \begin{bmatrix} \left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{21} & \alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) & \alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) + \alpha'_{xr} \frac{1}{\rho} r_\xi & 0 & 0 \end{bmatrix}$$

where

$$\left(\frac{\partial \hat{\mathbf{E}}_{\nu_1}}{\partial \hat{\mathbf{Q}}} \right)_{21} = -\alpha_{xx} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) - \alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) - \alpha'_{xr} \frac{v}{\rho} r_\xi$$

$$\alpha_{xx} = (2\mu + \lambda) \xi_x^2 + \mu \xi_r^2$$

$$\alpha_{xr} = (\mu + \lambda) \xi_x \xi_r$$

$$\alpha'_{xr} = \frac{\lambda}{r} \xi_x \xi_r$$

As in 2-D planar flow, the Jacobian coefficient matrices $\partial \hat{F}_2 / \partial \hat{Q}$ and $\partial (\hat{F}_{v1})_2 / \partial \hat{Q}$ have the same form as $\partial \hat{E}_2 / \partial \hat{Q}$ and $\partial (\hat{E}_{v1})_2 / \partial \hat{Q}$, but with ξ replaced by η .

Note that the equations for 2-D planar and axisymmetric flow are very similar. In the axisymmetric equations there are some additional terms involving the radius r in the viscous flux vectors, with corresponding terms in the Jacobian coefficient matrices. The radius r appears as an additional coefficient in front of the flux vectors \hat{E} , \hat{E}_{v1} , etc., and in front of the Jacobian coefficient matrices $\partial \hat{E}_2 / \partial \hat{Q}$, $\partial (\hat{E}_{v1})_2 / \partial \hat{Q}$, etc. In addition, $1/r$ appears in front of every term in the equation except the $\Delta(\rho u)$ terms. In *Proteus*, the Fortran variables are defined in such a way that, for many terms, the same coding can be used for both 2-D planar and axisymmetric flow. Unfortunately, this may make some of the coding a little confusing. It is hoped that this detailed description, when compared with the source listing, will help make things clear.

In COEFX, the coefficients of the left hand side, or implicit, terms are defined first. The implicit terms for the second ADI sweep have exactly the same form as for the first sweep, but with ξ replaced by η . By defining DEL, METX, METY, and METT as the grid spacing and metric coefficients in the sweep direction, the same coding can be used for both sweeps. The variable RAX is equal to 1 for 2-D planar flow, and the radius r for axisymmetric flow. This adds the r in front of the Jacobian coefficient matrices for axisymmetric flow, but has no effect for 2-D planar flow. The $1/r$ coefficient in front of each term will be added later. In this section of code, the coefficient of $\Delta(\rho u)$ (part of B(IV,I,NXM,NRU)) is set equal to r , not 1 as it should be. This will be corrected later.

The source term, or right hand side, for the first sweep is defined next. The difference formulas used to compute the source term are the same as those used for the implicit terms. These formulas are presented in Section 5.0 of Volume 1. For axisymmetric flow, the Fortran variable JI, which is normally defined as $1/J$, is temporarily redefined as r/J before the COEF routines are called. This automatically accounts for the r coefficient in front of all the flux vectors in the source term. The $1/r$ coefficient in front of each term will be added later. This definition of JI adds an r in front of the $\Delta(\rho u)^{n-1}$ term that should not be there. This will also be corrected later.

The coding for the source term for the second sweep, which consists only of $\Delta(\rho u)^*$, comes next. The definition of JI also adds an r in front of this term that should not be there.

And finally, for axisymmetric flow, the entire equation is divided by the local radius r . This adds the $1/r$ coefficient where it should be added, and removes the r in front of the $\Delta(\rho u)$ terms.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For sections of the code that apply to both sweeps (i.e., the implicit terms and the division by r at the end), the first two subscripts are written as (IV,I). For sections of the code that apply only to the first sweep, the first two subscripts are written as (I2,I1). For sections that apply only to the second sweep, they are written as (I1,I2). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.
3. The coding of the extra coefficients and source terms in the axisymmetric form of the equations is separate from the rest of the coding, and is bypassed if the flow is not axisymmetric. Similarly, the coding of coefficients and source terms involving the swirl velocity is separate from the rest of the coding, and is bypassed if there is no swirl.
4. The Euler option is implemented simply by skipping the calculation of the coefficients and source terms for the viscous terms.

5. The thin-layer option is implemented by skipping the calculation of the coefficients and source terms for the viscous terms containing derivatives in the specified direction.

Subroutine COEFY (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Compute coefficients and source term for the y or r -momentum equation.

Input

DEL	Computational grid spacing in sweep direction.
DPDRHO, DPDRU, DPDRV, DPDRW, DPDET	Derivatives $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, $\partial p/\partial(\rho v)$, $\partial p/\partial(\rho w)$, and $\partial p/\partial E_T$.
DTAU	Time step $\Delta \tau$.
DXI, DETA	Computational grid spacing $\Delta \xi$ and $\Delta \eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* IAXI	Flag for axisymmetric flow.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IEULER	Flag for Euler calculation.
* IHSTAG	Flag for constant stagnation enthalpy option.
ISWEEP	Current ADI sweep number.
* ISWIRL	Flag for swirl in axisymmetric flow.
* ITHIN	Flags for thin-layer option.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} (times the radius r for axisymmetric flow.)
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
MU, LA	Effective coefficient of viscosity μ and effective second coefficient of viscosity λ at time level n .
NEQ	Number of coupled equations being solved, N_{eq} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, METY, and METT.
NYM	Array index associated with the y -momentum (or r -momentum if axisymmetric) equation.
P	Static pressure p at time level n .
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w , at time level n .

RHOL, UL, VL	Static density ρ , and velocities u and v from previous ADI sweep.
* THY	Parameters θ_1 , θ_2 , and θ_3 determining type of time differencing for the y -momentum equation.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ , if axisymmetric), and ξ_r .
Y	Radial coordinate r for axisymmetric flow.

Output

A, B, C	Coefficient submatrices A, B, and C at interior points (row NYM only).
S	Source term subvector S at interior points (element NYM only).

Description

Subroutine COEFY computes the coefficients and source term for the y -momentum equation for 2-D planar flow, or the r -momentum equation for axisymmetric flow. Equations (7.5a-b) in Volume 1 represent, in vector form, the four governing difference equations for the two ADI sweeps for 2-D planar flow. The elements of the inviscid flux vectors $\hat{\mathbf{E}}$ and $\hat{\mathbf{F}}$ are given in Section 2.0 of Volume 1, and the elements of the viscous flux vectors $\hat{\mathbf{E}}_{\nu_1}$, $\hat{\mathbf{E}}_{\nu_2}$, etc., are given in Appendix A of Volume 1. The Jacobian coefficient matrices $\partial\hat{\mathbf{E}}/\partial\hat{\mathbf{Q}}$, $\partial\hat{\mathbf{E}}_{\nu_1}/\partial\hat{\mathbf{Q}}$, etc., are given in Section 4.0 of Volume 1. Using all of these equations, the differenced form of the y -momentum equation for 2-D planar flow may be written for the two ADI sweeps as²²

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta(\hat{\rho}v)_i^* + \frac{\theta_1 \Delta\tau}{(1+\theta_2)2\Delta\xi} \left[\left(\frac{\partial\hat{\mathbf{E}}_3}{\partial\hat{\mathbf{Q}}} \right)_{i+1}^n \Delta\hat{\mathbf{Q}}_{i+1}^* - \left(\frac{\partial\hat{\mathbf{E}}_3}{\partial\hat{\mathbf{Q}}} \right)_{i-1}^n \Delta\hat{\mathbf{Q}}_{i-1}^* \right] \\ - \frac{\theta_1 \Delta\tau}{(1+\theta_2)2(\Delta\xi)^2} \left[(f_{i-1} + f_i)^n g_{i-1}^n \Delta\hat{\mathbf{Q}}_{i-1}^* - (f_{i-1} + 2f_i + f_{i+1})^n g_i^n \Delta\hat{\mathbf{Q}}_i^* + (f_i + f_{i+1})^n g_{i+1}^n \Delta\hat{\mathbf{Q}}_{i+1}^* \right] = \\ - \frac{\Delta\tau}{1+\theta_2} (\delta_\xi \hat{\mathbf{E}}_3 + \delta_\eta \hat{\mathbf{F}}_3)^n + \frac{\Delta\tau}{1+\theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_1})_3 + \delta_\eta (\hat{\mathbf{F}}_{\nu_1})_3]^n \\ + \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_2})_3 + \delta_\eta (\hat{\mathbf{F}}_{\nu_2})_3]^n - \frac{\theta_3 \Delta\tau}{1+\theta_2} [\delta_\xi (\hat{\mathbf{E}}_{\nu_2})_3 + \delta_\eta (\hat{\mathbf{F}}_{\nu_2})_3]^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta(\hat{\rho}v)^{n-1} \end{aligned}$$

²² These equations are written assuming the energy equation is being solved. For a constant stagnation enthalpy case, the total energy E_T would not appear as a dependent variable, and the Jacobian coefficient matrices would have only three elements.

Sweep 2 (η direction)

$$\Delta(\hat{\rho}v)_j^n + \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 \Delta \eta} \left[\left(\frac{\partial \hat{F}_3}{\partial \hat{Q}} \right)_{j+1}^n \Delta \hat{Q}_{j+1}^n - \left(\frac{\partial \hat{F}_3}{\partial \hat{Q}} \right)_{j-1}^n \Delta \hat{Q}_{j-1}^n \right] - \frac{\theta_1 \Delta \tau}{(1 + \theta_2) 2 (\Delta \eta)^2} \left[(f_{j-1} + f_j)^n g_{j-1}^n \Delta \hat{Q}_{j-1}^n - (f_{j-1} + 2f_j + f_{j+1})^n g_j^n \Delta \hat{Q}_j^n + (f_j + f_{j+1})^n g_{j+1}^n \Delta \hat{Q}_{j+1}^n \right] = \Delta(\hat{\rho}v)^*$$

In the above equations, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j . On the left hand side, f is the coefficient of $\partial/\partial \xi$ (or $\partial/\partial \eta$, depending on the sweep) in the $\partial \hat{E}_{v1}/\partial \hat{Q}$ (or $\partial \hat{F}_{v1}/\partial \hat{Q}$) Jacobian coefficient matrix. Similarly, g is the term in the parentheses following $\partial/\partial \xi$ (or $\partial/\partial \eta$) in the $\partial \hat{E}_{v1}/\partial \hat{Q}$ (or $\partial \hat{F}_{v1}/\partial \hat{Q}$) Jacobian coefficient matrix.

The vector of dependent variables is

$$\hat{Q} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad E_T]^T$$

The appropriate elements of the inviscid flux vectors are given by

$$\begin{aligned} \hat{E}_3 &= \frac{1}{J} [\rho u v \xi_x + (\rho v^2 + p) \xi_y + \rho v \xi_t] \\ \hat{F}_3 &= \frac{1}{J} [\rho u v \eta_x + (\rho v^2 + p) \eta_y + \rho v \eta_t] \end{aligned}$$

The appropriate elements of the non-cross derivative viscous flux vectors are

$$\begin{aligned} (\hat{E}_{v1})_3 &= \frac{1}{J} \frac{1}{Re_r} [2\mu \xi_y^2 v_\xi + \lambda \xi_y (\xi_x u_\xi + \xi_y v_\xi) + \mu \xi_x (\xi_y u_\xi + \xi_x v_\xi)] \\ (\hat{F}_{v1})_3 &= \frac{1}{J} \frac{1}{Re_r} [2\mu \eta_y^2 v_\eta + \lambda \eta_y (\eta_x u_\eta + \eta_y v_\eta) + \mu \eta_x (\eta_y u_\eta + \eta_x v_\eta)] \end{aligned}$$

And the appropriate elements of the cross derivative viscous flux vectors are

$$\begin{aligned} (\hat{E}_{v2})_3 &= \frac{1}{J} \frac{1}{Re_r} [2\mu \xi_y \eta_y v_\eta + \lambda \xi_y (\eta_x u_\eta + \eta_y v_\eta) + \mu \xi_x (\eta_y u_\eta + \eta_x v_\eta)] \\ (\hat{F}_{v2})_3 &= \frac{1}{J} \frac{1}{Re_r} [2\mu \eta_y \xi_y v_\xi + \lambda \eta_y (\xi_x u_\xi + \xi_y v_\xi) + \mu \eta_x (\xi_y u_\xi + \xi_x v_\xi)] \end{aligned}$$

The elements of the Jacobian coefficient matrix $\partial \hat{E}/\partial \hat{Q}$ for the inviscid terms in the y -momentum equation are

$$\frac{\partial \hat{E}_3}{\partial \hat{Q}} = \begin{bmatrix} \frac{\partial p}{\partial \rho} \xi_y - v f_1 & v \xi_x + \frac{\partial p}{\partial (\rho u)} \xi_y & \xi_t + f_1 + v \xi_y + \frac{\partial p}{\partial (\rho v)} \xi_y & \frac{\partial p}{\partial E_T} \xi_y \end{bmatrix}$$

where $f_1 = u \xi_x + v \xi_y$.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}}_{v_1} / \partial \hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial (\hat{\mathbf{E}}_{v_1})_3}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial \hat{\mathbf{E}}_{v_1}}{\partial \hat{\mathbf{Q}}} \right)_{31} \quad \alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) \quad \alpha_{yy} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) \quad 0 \right]$$

where

$$\left(\frac{\partial \hat{\mathbf{E}}_{v_1}}{\partial \hat{\mathbf{Q}}} \right)_{31} = -\alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) - \alpha_{yy} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right)$$

$$\alpha_{xy} = (\mu + \lambda) \xi_x \xi_y$$

$$\alpha_{yy} = \mu \xi_x^2 + (2\mu + \lambda) \xi_y^2$$

The Jacobian coefficient matrices $\partial \hat{\mathbf{F}}_3 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{F}}_{v_1})_3 / \partial \hat{\mathbf{Q}}$ have the same form as $\partial \hat{\mathbf{E}}_3 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{E}}_{v_1})_3 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

As an example of how these equations are translated into Fortran, consider the $\Delta(\rho u/J)$ term on the left hand side for the first sweep. This is the second element of $\hat{\mathbf{Q}}$, so using the second element in $\partial \hat{\mathbf{E}}_3 / \partial \hat{\mathbf{Q}}$, we get for the inviscid term

$$A(\text{IV}, \text{I}, \text{NYM}, \text{NRU}) = -\frac{\theta_1(\Delta\tau)_{i,j}}{(1 + \theta_2)2\Delta\xi} \left[(v\xi_x)_{i-1,j} + \left(\frac{\partial p}{\partial(\rho u)} \xi_y \right)_{i-1,j} \right]$$

$$B(\text{IV}, \text{I}, \text{NYM}, \text{NRU}) = 0$$

$$C(\text{IV}, \text{I}, \text{NYM}, \text{NRU}) = \frac{\theta_1(\Delta\tau)_{i,j}}{(1 + \theta_2)2\Delta\xi} \left[(v\xi_x)_{i+1,j} + \left(\frac{\partial p}{\partial(\rho u)} \xi_y \right)_{i+1,j} \right]$$

For the viscous terms on the left hand side, we use the second element in $\partial (\hat{\mathbf{E}}_{v_1})_3 / \partial \hat{\mathbf{Q}}$, which is

$$\frac{1}{Re_r} \alpha_{xy} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right)$$

Thus $f = \alpha_{xy}/Re_r$, and $g = 1/\rho$. To add the viscous contribution to this part of the **A** coefficient submatrix, we therefore set

$$A(\text{IV}, \text{I}, \text{NYM}, \text{NRU}) = A(\text{IV}, \text{I}, \text{NYM}, \text{NRU}) - \frac{\theta_1(\Delta\tau)_{i,j}}{(1 + \theta_2)2(\Delta\xi)^2 Re_r} [(\alpha_{xy})_{i-1,j} + (\alpha_{xy})_{i,j}] \left(\frac{1}{\rho} \right)_{i-1,j}$$

Similar equations may be written for the **B** and **C** coefficient submatrices.

The equations for axisymmetric flow are developed in Appendix B of Volume 1. The axisymmetric r -momentum equation for the two ADI sweeps is given by²³

²³ These equations are written for the general case with swirl. For a non-swirl case, the swirl momentum ρw would not appear as a dependent variable, and the Jacobian coefficient matrices would have only four elements.

Sweep 1 (ξ direction)

$$\begin{aligned}
\Delta(\hat{\rho}v)_i^* + \frac{\theta_1 \Delta \tau}{(1+\theta_2)2\Delta\xi} \frac{1}{r} \left[\left(r \frac{\partial \hat{E}_3}{\partial \hat{Q}} \right)_{i+1}^n \Delta \hat{Q}_{i+1}^* - \left(r \frac{\partial \hat{E}_3}{\partial \hat{Q}} \right)_{i-1}^n \Delta \hat{Q}_{i-1}^* \right] \\
- \frac{\theta_1 \Delta \tau}{(1+\theta_2)2(\Delta\xi)^2} \frac{1}{r} \left[(r_{i-1}f_{i-1} + r_i f_i)^n g_{i-1}^n \Delta \hat{Q}_{i-1}^* - (r_{i-1}f_{i-1} + 2r_i f_i + r_{i+1}f_{i+1})^n g_i^n \Delta \hat{Q}_i^* + (r_i f_i + r_{i+1}f_{i+1})^n g_{i+1}^n \Delta \hat{Q}_{i+1}^* \right] \\
+ \frac{\theta_1 \Delta \tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial \hat{H}_3}{\partial \hat{Q}} - \frac{\partial(\hat{H}v)_3}{\partial \hat{Q}} \right]_i \Delta \hat{Q}_i^* = -\frac{\Delta \tau}{1+\theta_2} \frac{1}{r} \left[\delta_\xi(r \hat{E}_3) + \delta_\eta(r \hat{F}_3) + \hat{H}_3 \right]^n \\
+ \frac{\Delta \tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}v)_3] + \delta_\eta[r(\hat{F}v)_3] + (\hat{H}v)_3 \right\}^n + \frac{(1+\theta_3)\Delta \tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}v)_3] + \delta_\eta[r(\hat{F}v)_3] \right\}^n \\
- \frac{\theta_3 \Delta \tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}v)_3] + \delta_\eta[r(\hat{F}v)_3] \right\}^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta(\hat{\rho}v)^{n-1}
\end{aligned}$$

Sweep 2 (η direction)

$$\begin{aligned}
\Delta(\hat{\rho}v)_j^n + \frac{\theta_1 \Delta \tau}{(1+\theta_2)2\Delta\eta} \frac{1}{r} \left[\left(r \frac{\partial \hat{F}_3}{\partial \hat{Q}} \right)_{j+1}^n \Delta \hat{Q}_{j+1}^n - \left(r \frac{\partial \hat{F}_3}{\partial \hat{Q}} \right)_{j-1}^n \Delta \hat{Q}_{j-1}^n \right] \\
- \frac{\theta_1 \Delta \tau}{(1+\theta_2)2(\Delta\eta)^2} \frac{1}{r} \left[(r_{j-1}f_{j-1} + r_j f_j)^n g_{j-1}^n \Delta \hat{Q}_{j-1}^n - (r_{j-1}f_{j-1} + 2r_j f_j + r_{j+1}f_{j+1})^n g_j^n \Delta \hat{Q}_j^n + (r_j f_j + r_{j+1}f_{j+1})^n g_{j+1}^n \Delta \hat{Q}_{j+1}^n \right] \\
+ \frac{\theta_1 \Delta \tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial \hat{H}_3}{\partial \hat{Q}} - \frac{\partial(\hat{H}v)_3}{\partial \hat{Q}} \right]_j \Delta \hat{Q}_j^n = \\
\Delta(\hat{\rho}v)^* + \frac{\theta_1 \Delta \tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial \hat{H}_3}{\partial \hat{Q}} - \frac{\partial(\hat{H}v)_3}{\partial \hat{Q}} \right] \Delta \hat{Q}^*
\end{aligned}$$

where now

$$\hat{Q} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T$$

$$\hat{E}_3 = \frac{1}{J} [\rho u v \xi_x + (\rho v^2 + p) \xi_r + \rho v \xi_t]$$

$$\hat{F}_3 = \frac{1}{J} [\rho u v \eta_x + (\rho v^2 + p) \eta_r + \rho v \eta_t]$$

$$(\hat{E}v)_3 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \xi_r^2 v_\xi + \lambda \xi_r \left[\xi_x u_\xi + \frac{1}{r} \xi_r (rv)_\xi \right] + \mu \xi_x (\xi_r u_\xi + \xi_x v_\xi) \right\}$$

$$(\hat{F}v)_3 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \eta_r^2 v_\eta + \lambda \eta_r \left[\eta_x u_\eta + \frac{1}{r} \eta_r (rv)_\eta \right] + \mu \eta_x (\eta_r u_\eta + \eta_x v_\eta) \right\}$$

$$(\hat{E}v)_3 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \xi_r \eta_r v_\eta + \lambda \xi_r \left[\eta_x u_\eta + \frac{1}{r} \eta_r (rv)_\eta \right] + \mu \xi_x (\eta_r u_\eta + \eta_x v_\eta) \right\}$$

$$(\hat{F}v)_3 = \frac{1}{J} \frac{1}{Re_r} \left\{ 2\mu \eta_r \xi_r v_\xi + \lambda \eta_r \left[\xi_x u_\xi + \frac{1}{r} \xi_r (rv)_\xi \right] + \mu \eta_x (\xi_r u_\xi + \xi_x v_\xi) \right\}$$

$$\hat{H}_3 = \frac{1}{J} (-p - \rho w^2)$$

$$(\hat{\mathbf{H}}_\nu)_3 = \frac{1}{J} \frac{1}{Re_r} \left\{ -2\mu \frac{v}{r} - \lambda(\xi_x u_\xi + \eta_x u_\eta) + \frac{\lambda}{r} [\xi_r(rv)_\xi + \eta_r(rv)_\eta] \right\}$$

The $\hat{\mathbf{H}}$ and $\hat{\mathbf{H}}_\nu$ terms, which do not appear in the 2-D planar form of the equations, result from the non-conservative form of the axisymmetric equations.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}} / \partial \hat{\mathbf{Q}}$ for the inviscid terms in the axisymmetric form of the energy equation are

$$\frac{\partial \hat{\mathbf{E}}_3}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} \frac{\partial p}{\partial \rho} \xi_r - v f_1 & v \xi_x + \frac{\partial p}{\partial(\rho u)} \xi_r & \xi_t + f_1 + v \xi_r + \frac{\partial p}{\partial(\rho v)} \xi_r & \frac{\partial p}{\partial(\rho w)} \xi_r & \frac{\partial p}{\partial E_T} \xi_r \end{bmatrix}$$

where $f_1 = u \xi_x + v \xi_r$.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}}_\nu / \partial \hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial (\hat{\mathbf{E}}_\nu)_3}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial \hat{\mathbf{E}}_\nu}{\partial \hat{\mathbf{Q}}} \right)_{31} \quad \alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) \quad \alpha_{rr} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) + \alpha'_{rr} \frac{1}{\rho} r_\xi \quad 0 \quad 0 \right]$$

where

$$\left(\frac{\partial \hat{\mathbf{E}}_\nu}{\partial \hat{\mathbf{Q}}} \right)_{31} = -\alpha_{xr} \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) - \alpha_{rr} \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) - \alpha'_{rr} \frac{v}{\rho} r_\xi$$

$$\alpha_{xr} = (\mu + \lambda) \xi_x \xi_r$$

$$\alpha_{rr} = \mu \xi_x^2 + (2\mu + \lambda) \xi_r^2$$

$$\alpha'_{rr} = \frac{\lambda}{r} \xi_r^2$$

As in 2-D planar flow, the Jacobian coefficient matrices $\partial \hat{\mathbf{F}}_3 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{F}}_\nu)_3 / \partial \hat{\mathbf{Q}}$ have the same form as $\partial \hat{\mathbf{E}}_3 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{E}}_\nu)_3 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{H}} / \partial \hat{\mathbf{Q}}$ are

$$\frac{\partial \hat{\mathbf{H}}_3}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} -\frac{\partial p}{\partial \rho} + w^2 & -\frac{\partial p}{\partial(\rho u)} & -\frac{\partial p}{\partial(\rho v)} & -\frac{\partial p}{\partial(\rho w)} - 2w & -\frac{\partial p}{\partial E_T} \end{bmatrix}$$

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{H}}_\nu / \partial \hat{\mathbf{Q}}$ are

$$\frac{\partial (\hat{\mathbf{H}}_\nu)_3}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial \hat{\mathbf{H}}_\nu}{\partial \hat{\mathbf{Q}}} \right)_{31} \quad \left(\frac{\partial \hat{\mathbf{H}}_\nu}{\partial \hat{\mathbf{Q}}} \right)_{32} \quad \left(\frac{\partial \hat{\mathbf{H}}_\nu}{\partial \hat{\mathbf{Q}}} \right)_{33} \quad 0 \quad 0 \right]$$

where

$$\begin{aligned}
\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{31} &= \lambda \xi_x \frac{\partial}{\partial \xi} \left(\frac{u}{\rho} \right) + \lambda \xi_r \frac{\partial}{\partial \xi} \left(\frac{v}{\rho} \right) + \lambda \eta_x \frac{\partial}{\partial \eta} \left(\frac{u}{\rho} \right) \\
&\quad + [2\mu + \lambda(\xi_r r_\xi + \eta_r r_\eta)] \frac{1}{r} \frac{v}{\rho} + \lambda \eta_r \frac{\partial}{\partial \eta} \left(\frac{v}{\rho} \right) \\
\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{32} &= -\lambda \xi_x \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) - \lambda \eta_x \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \\
\left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{33} &= -\lambda \xi_r \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) - [2\mu + \lambda(\xi_r r_\xi + \eta_r r_\eta)] \frac{1}{r} \frac{1}{\rho} - \lambda \eta_r \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right)
\end{aligned}$$

Note that, except for the additional $\hat{\mathbf{H}}$ and $\hat{\mathbf{H}}_V$ terms, the equations for 2-D planar and axisymmetric flow are very similar. In the axisymmetric equations there are some additional terms involving the radius r in the viscous flux vectors, with corresponding terms in the Jacobian coefficient matrices. The radius r appears as an additional coefficient in front of the flux vectors $\hat{\mathbf{E}}$, $\hat{\mathbf{E}}_V$, etc., and in front of the Jacobian coefficient matrices $\partial \hat{\mathbf{E}}_3 / \partial \hat{\mathbf{Q}}$, $\partial (\hat{\mathbf{E}}_V)_3 / \partial \hat{\mathbf{Q}}$, etc. In addition, $1/r$ appears in front of every term in the equation except the $\Delta(\hat{\rho}v)$ terms. In *Proteus*, the Fortran variables are defined in such a way that, for many terms, the same coding can be used for both 2-D planar and axisymmetric flow. Unfortunately, this may make some of the coding a little confusing. It is hoped that this detailed description, when compared with the source listing, will help make things clear.

In COEFY, the coefficients of the left hand side, or implicit, terms are defined first. Note that the implicit terms for the second ADI sweep have exactly the same form as for the first sweep, but with ξ replaced by η . By defining DEL, METX, METY, and METT as the grid spacing and metric coefficients in the sweep direction, the same coding can be used for both sweeps. The variable RAX is equal to 1 for 2-D planar flow, and the radius r for axisymmetric flow. This adds the r in front of the Jacobian coefficient matrices for axisymmetric flow, but has no effect for 2-D planar flow. The $1/r$ coefficient in front of each term will be added later. In this section of code, the coefficient of $\Delta(\hat{\rho}v)$ (part of B(IV,I,NYM,NRV)) is set equal to r , not 1 as it should be. This will be corrected later.

The source term, or right hand side, for the first sweep is defined next. The difference formulas used to compute the source term are the same as those used for the implicit terms. These formulas are presented in Section 5.0 of Volume 1. For axisymmetric flow, the Fortran variable JI, which is normally defined as $1/J$, is temporarily redefined as r/J before the COEF routines are called. This automatically accounts for the r coefficient in front of all the flux vectors in the source term. The $1/r$ coefficient in front of each term will be added later. This definition of JI adds an r in front of the $\Delta(\hat{\rho}v)^{n-1}$ term that should not be there. This will also be corrected later.

The coding for the source term for the second sweep comes next. The definition of JI also adds an r in front of the $\Delta(\hat{\rho}v)^*$ term that should not be there.

And finally, for axisymmetric flow, the entire equation is divided by the local radius r . This adds the $1/r$ coefficient where it should be added, and removes the r in front of the $\Delta(\hat{\rho}v)$ terms.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For sections of the code that apply to both sweeps (i.e., the implicit terms and the division by r at the end), the first two subscripts are written as (IV,I). For sections of the code that apply only

to the first sweep, the first two subscripts are written as (I2,I1). For sections that apply only to the second sweep, they are written as (I1,I2). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.

3. The coding of the extra coefficients and source terms in the axisymmetric form of the equations is separate from the rest of the coding, and is bypassed if the flow is not axisymmetric. Similarly, the coding of coefficients and source terms involving the swirl velocity is separate from the rest of the coding, and is bypassed if there is no swirl.
4. The Euler option is implemented simply by skipping the calculation of the coefficients and source terms for the viscous terms.
5. The thin-layer option is implemented by skipping the calculation of the coefficients and source terms for the viscous terms containing derivatives in the specified direction.

Subroutine COEFZ (A,B,C,S,METX,METY,METT,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Compute coefficients and source term for the swirl momentum equation.

Input

DEL	Computational grid spacing in sweep direction.
DTAU	Time step $\Delta\tau$.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IEULER	Flag for Euler calculation.
* IHSTAG	Flag for constant stagnation enthalpy option.
ISWEEP	Current ADI sweep number.
* ITHIN	Flags for thin-layer option.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation times the radius, rJ^{-1} .
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , r , and t .
MU	Effective coefficient of viscosity μ at time level n .
NEQ	Number of coupled equations being solved, N_{eq} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, S, METX, METY, and METT.
NZM	Array index associated with the swirl momentum equation.
RAX	The local radius r .
* RER	Reference Reynolds number Re_r .
RHO, U, V, W	Static density ρ , and velocities u , v , and w , at time level n .
RHOL, WL	Static density ρ and velocity w from previous ADI sweep.
* THZ	Parameters θ_1 , θ_2 , and θ_3 determining type of time differencing for the swirl momentum equation.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .
Y	Radial coordinate r .

Output

A, B, C

Coefficient submatrices A, B, and C at interior points (row NZM only).

S

Source term subvector S at interior points (element NZM only).

Description

Subroutine COEFZ computes the coefficients and source term for the swirl momentum equation, which is only valid in axisymmetric flow. The equations for axisymmetric flow are developed in Appendix B of Volume 1. The swirl momentum equation for the two ADI sweeps is given by²⁴

Sweep 1 (ξ direction)

$$\begin{aligned} \Delta(\rho\hat{w})_i^* + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\xi} \frac{1}{r} \left[\left(r \frac{\partial\hat{E}_4}{\partial\hat{Q}} \right)_{i+1}^n \Delta\hat{Q}_{i+1}^* - \left(r \frac{\partial\hat{E}_4}{\partial\hat{Q}} \right)_{i-1}^n \Delta\hat{Q}_{i-1}^* \right] \\ - \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\xi)^2} \frac{1}{r} \left[(r_{i-1}f_{i-1} + r_i f_i)^n g_{i-1}^n \Delta\hat{Q}_{i-1}^* - (r_{i-1}f_{i-1} + 2r_i f_i + r_{i+1}f_{i+1})^n g_i^n \Delta\hat{Q}_i^* + (r_i f_i + r_{i+1}f_{i+1})^n g_{i+1}^n \Delta\hat{Q}_{i+1}^* \right] \\ + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial\hat{H}_4}{\partial\hat{Q}} - \frac{\partial(\hat{H}_v)_4}{\partial\hat{Q}} \right]_i^n \Delta\hat{Q}_i^* = - \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\delta_\xi(r\hat{E}_4) + \delta_\eta(r\hat{F}_4) + \hat{H}_4 \right]^n + \frac{\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_1})_4] + \delta_\eta[r(\hat{F}_{v_1})_4] + (\hat{H}_{v_1})_4 \right\}^n \\ + \frac{(1+\theta_3)\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_2})_4] + \delta_\eta[r(\hat{F}_{v_2})_4] \right\}^n - \frac{\theta_3\Delta\tau}{1+\theta_2} \frac{1}{r} \left\{ \delta_\xi[r(\hat{E}_{v_2})_4] + \delta_\eta[r(\hat{F}_{v_2})_4] \right\}^{n-1} + \frac{\theta_2}{1+\theta_2} \Delta(\rho\hat{w})^{n-1} \end{aligned}$$

Sweep 2 (η direction)

$$\begin{aligned} \Delta(\rho\hat{w})_j^n + \frac{\theta_1\Delta\tau}{(1+\theta_2)2\Delta\eta} \frac{1}{r} \left[\left(r \frac{\partial\hat{F}_4}{\partial\hat{Q}} \right)_{j-1}^n \Delta\hat{Q}_{j-1}^n - \left(r \frac{\partial\hat{F}_4}{\partial\hat{Q}} \right)_{j+1}^n \Delta\hat{Q}_{j+1}^n \right] \\ - \frac{\theta_1\Delta\tau}{(1+\theta_2)2(\Delta\eta)^2} \frac{1}{r} \left[(r_{j-1}f_{j-1} + r_j f_j)^n g_{j-1}^n \Delta\hat{Q}_{j-1}^n - (r_{j-1}f_{j-1} + 2r_j f_j + r_{j+1}f_{j+1})^n g_j^n \Delta\hat{Q}_j^n + (r_j f_j + r_{j+1}f_{j+1})^n g_{j+1}^n \Delta\hat{Q}_{j+1}^n \right] \\ + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial\hat{H}_4}{\partial\hat{Q}} - \frac{\partial(\hat{H}_v)_4}{\partial\hat{Q}} \right]_j^n \Delta\hat{Q}_j^n = \Delta(\rho\hat{w})^* + \frac{\theta_1\Delta\tau}{1+\theta_2} \frac{1}{r} \left[\frac{\partial\hat{H}_4}{\partial\hat{Q}} - \frac{\partial(\hat{H}_v)_4}{\partial\hat{Q}} \right] \Delta\hat{Q}^* \end{aligned}$$

In the above equations, the subscripts i and j represent grid point indices in the ξ and η directions. For notational convenience, terms without an explicitly written i or j subscript are understood to be at i or j . On the left hand side, f is the coefficient of $\partial/\partial\xi$ (or $\partial/\partial\eta$, depending on the sweep) in the $\partial\hat{E}_{v_1}/\partial\hat{Q}$ (or $\partial\hat{F}_{v_1}/\partial\hat{Q}$) Jacobian coefficient matrix. Similarly, g is the term in the parentheses following $\partial/\partial\xi$ (or $\partial/\partial\eta$) in the $\partial\hat{E}_{v_1}/\partial\hat{Q}$ (or $\partial\hat{F}_{v_1}/\partial\hat{Q}$) Jacobian coefficient matrix.

The vector of dependent variables is

$$\hat{Q} = \frac{1}{J} [\rho \quad \rho u \quad \rho v \quad \rho w \quad E_T]^T$$

The appropriate elements of the inviscid flux vectors are given by

²⁴ These equations are written assuming the energy equation is being solved. For a constant stagnation enthalpy case, the total energy E_T would not appear as a dependent variable, and the Jacobian coefficient matrices would have only four elements.

$$\hat{\mathbf{E}}_4 = \frac{1}{J} [\rho u w \xi_x + \rho v w \xi_r + \rho w \xi_t]$$

$$\hat{\mathbf{F}}_4 = \frac{1}{J} [\rho u w \eta_x + \rho v w \eta_r + \rho w \eta_t]$$

The appropriate elements of the non-cross derivative viscous flux vectors are

$$(\hat{\mathbf{E}}_{V_1})_4 = \frac{1}{J} \frac{1}{Re_r} (\mu \xi_x^2 w_\xi + \mu \xi_r^2 w_\xi)$$

$$(\hat{\mathbf{F}}_{V_1})_4 = \frac{1}{J} \frac{1}{Re_r} (\mu \eta_x^2 w_\eta + \mu \eta_r^2 w_\eta)$$

And the appropriate elements of the cross derivative viscous flux vectors are

$$(\hat{\mathbf{E}}_{V_2})_4 = \frac{1}{J} \frac{1}{Re_r} (\mu \xi_x \eta_x w_\eta + \mu \xi_r \eta_r w_\eta - \mu \xi_r \frac{w}{r})$$

$$(\hat{\mathbf{F}}_{V_2})_4 = \frac{1}{J} \frac{1}{Re_r} (\mu \eta_x \xi_x w_\xi + \mu \eta_r \xi_r w_\xi - \mu \eta_r \frac{w}{r})$$

The extra terms resulting from the non-conservative form of the axisymmetric equations are

$$\hat{\mathbf{H}}_4 = \frac{1}{J} \rho v w$$

$$(\hat{\mathbf{H}}_V)_4 = \frac{1}{J} \frac{1}{Re_r} \left[\mu (\xi_r w_\xi + \eta_r w_\eta) - \mu \frac{w}{r} \right]$$

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}} / \partial \hat{\mathbf{Q}}$ for the inviscid terms in the r -momentum equation are

$$\frac{\partial \hat{\mathbf{E}}_4}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} -w f_1 & w \xi_x & w \xi_r & \xi_t + f_1 & 0 \end{bmatrix}$$

where $f_1 = u \xi_x + v \xi_r$.

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{E}}_{V_1} / \partial \hat{\mathbf{Q}}$ for the viscous terms are

$$\frac{\partial (\hat{\mathbf{E}}_{V_1})_4}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \left[\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{41} \quad 0 \quad 0 \quad \alpha_{zz} \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) \quad 0 \right]$$

where

$$\left(\frac{\partial \hat{\mathbf{E}}_{V_1}}{\partial \hat{\mathbf{Q}}} \right)_{41} = -\alpha_{zz} \frac{\partial}{\partial \xi} \left(\frac{w}{\rho} \right)$$

$$\alpha_{zz} = \mu \xi_x^2 + \mu \xi_r^2$$

The Jacobian coefficient matrices $\partial \hat{\mathbf{F}}_4 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{F}}_{V_1})_4 / \partial \hat{\mathbf{Q}}$ have the same form as $\partial \hat{\mathbf{E}}_4 / \partial \hat{\mathbf{Q}}$ and $\partial (\hat{\mathbf{E}}_{V_1})_4 / \partial \hat{\mathbf{Q}}$, but with ξ replaced by η .

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{H}} / \partial \hat{\mathbf{Q}}$ are

$$\frac{\partial \hat{\mathbf{H}}_4}{\partial \hat{\mathbf{Q}}} = \begin{bmatrix} -vw & 0 & w & v & 0 \end{bmatrix}$$

The elements of the Jacobian coefficient matrix $\partial \hat{\mathbf{H}}_V / \partial \hat{\mathbf{Q}}$ are

$$\frac{\partial (\hat{\mathbf{H}}_V)_4}{\partial \hat{\mathbf{Q}}} = \frac{1}{Re_r} \begin{bmatrix} \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{41} & 0 & 0 & \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{44} & 0 \end{bmatrix}$$

where

$$\begin{aligned} \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{41} &= -\mu \xi_r \frac{\partial}{\partial \xi} \left(\frac{w}{\rho} \right) + \frac{\mu}{r} \frac{w}{\rho} - \mu \eta_r \frac{\partial}{\partial \eta} \left(\frac{w}{\rho} \right) \\ \left(\frac{\partial \hat{\mathbf{H}}_V}{\partial \hat{\mathbf{Q}}} \right)_{44} &= \mu \xi_r \frac{\partial}{\partial \xi} \left(\frac{1}{\rho} \right) - \frac{\mu}{r} \frac{1}{\rho} + \mu \eta_r \frac{\partial}{\partial \eta} \left(\frac{1}{\rho} \right) \end{aligned}$$

As an example of how these equations are translated into Fortran, consider the $\Delta(\rho v/J)$ term on the left hand side for the first sweep. This is the third element of $\hat{\mathbf{Q}}$, so using the third element in $\partial \hat{\mathbf{E}}_4 / \partial \hat{\mathbf{Q}}$, and including the contribution from the third element of $\partial \hat{\mathbf{H}}_4 / \partial \hat{\mathbf{Q}}$, we get for the inviscid term

$$\begin{aligned} A(\text{IV}, \text{I}, \text{NZM}, \text{NRV}) &= -\frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \frac{1}{r_{i,j}} [(rw\xi_r)_{i-1,j}] \\ B(\text{IV}, \text{I}, \text{NZM}, \text{NRV}) &= \frac{\theta_1(\Delta\tau)_{i,j}}{1+\theta_2} \frac{1}{r_{i,j}} w_{i,j} \\ C(\text{IV}, \text{I}, \text{NZM}, \text{NRV}) &= \frac{\theta_1(\Delta\tau)_{i,j}}{(1+\theta_2)2\Delta\xi} \frac{1}{r_{i,j}} [(rw\xi_r)_{i+1,j}] \end{aligned}$$

For the $\Delta(\rho v/J)$ term, there are no viscous terms on the left hand side.

In COEFZ, the coefficients of the left hand side, or implicit, terms are defined first. Note that the implicit terms for the second sweep have exactly the same form as for the first sweep, but with ξ replaced by η . By defining DEL, METX, METY, and METT as the grid spacing and metric coefficients in the sweep direction, the same coding can be used for both sweeps. Since COEFZ is only used in axisymmetric flow, the variable RAX is equal to the radius r . This adds the r in front of the Jacobian coefficient matrices. The $1/r$ coefficient in front of each term will be added later. In this section of code, the coefficient of $\Delta(\rho w)$ (part of $B(\text{IV}, \text{I}, \text{NZM}, \text{NRW})$) is set equal to r , not 1 as it should be. This will be corrected later.

The source term, or right hand side, for the first sweep is defined next. The difference formulas used to compute the source term are the same as those used for the implicit terms. These formulas are presented in Section 5.0 of Volume 1. For axisymmetric flow, the Fortran variable JI, which is normally defined as $1/J$, is temporarily redefined as r/J before the COEF routines are called. This automatically accounts for the r coefficient in front of all the flux vectors in the source term. The $1/r$ coefficient in front of each term will be added later. This definition of JI adds an r in front of the $\Delta(\rho w)^{n-1}$ term that should not be there. This will also be corrected later.

The coding for the source term for the second sweep comes next. The definition of JI also adds an r in front of the $\Delta(\rho\hat{w})^*$ term that should not be there.

And finally, the entire equation is divided by the local radius r . This adds the $1/r$ coefficient where it should be added, and removes the r in front of the $\Delta(\rho\hat{w})$ terms.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.
2. The subscripts on the Fortran variables A, B, C, and S may be confusing. The first subscript is the index in the non-sweep (i.e., "vectorized") direction, and the second subscript is the index in the sweep direction. For sections of the code that apply to both sweeps (i.e., the implicit terms and the division by r at the end), the first two subscripts are written as (IV,I). For sections of the code that apply only to the first sweep, the first two subscripts are written as (I2,I1). For sections that apply only to the second sweep, they are written as (I1,I2). The third subscript on A, B, C, and S corresponds to the equation. And, for A, B, and C, the fourth subscript corresponds to the dependent variable for which A, B, or C is a coefficient.
3. The coding of the extra coefficients and source terms in the axisymmetric form of the equations is separate from the rest of the coding, and is bypassed if the flow is not axisymmetric. Similarly, the coding of coefficients and source terms involving the swirl velocity is separate from the rest of the coding, and is bypassed if there is no swirl.
4. The Euler option is implemented simply by skipping the calculation of the coefficients and source terms for the viscous terms.
5. The thin-layer option is implemented by skipping the calculation of the coefficients and source terms for the viscous terms containing derivatives in the specified direction.

Subroutine CONV		
Called by	Calls	Purpose
MAIN	ISAMAX	Test computed flow field for convergence.

Input

CHGMAX	Maximum change in absolute value of the dependent variables from time level $n - 1$ to n (or over the previous NITAVG - 1 time steps if ICTEST = 2), ΔQ_{max} .
DUMMY	A two-dimensional scratch array.
* EPS	Convergence level to be reached, ε .
* GAMR	Reference ratio of specific heats, γ_r .
* IAV2E, IAV4E	Flags for second- and fourth-order explicit implicit artificial viscosity.
* ICTEST	Flag for convergence criteria to be used.
* IHSTAG	Flag for constant stagnation enthalpy option.
* ISWIRL	Flag for swirl in axisymmetric flow.
IT	Current time step number n .
NEQ	Number of coupled equations being solved, N_{eq} .
* NITAVG	Number of time steps in moving average convergence test.
* NOUT	Unit number for standard output.
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NTOTP	Dimensioning parameter specifying the storage required for a full two-dimensional array (i.e., $N1P \times N2P$).
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
RESAVG	The average absolute value of the residual at time level n , R_{avg} .
RESL2	The L_2 norm of the residual at time level n , R_{L_2} .
RESMAX	The maximum absolute value of the residual at time level n , R_{max} .
RGAS	Gas constant R .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level $n + 1$.
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .

Output

CHGAVG	Maximum change in absolute value of the dependent variables, averaged over the last NITAVG time steps, ΔQ_{avg} .
CHGMAX	Maximum change in absolute value of the dependent variables from time level n to $n + 1$ (or over the previous NITAVG time steps if ICTEST = 2), ΔQ_{max} .

ICONV

Convergence flag; 1 if converged, 0 if not.

Description

Subroutine CONV checks the computed flow field for convergence. Convergence may be based on: (1) the absolute value of the maximum change in the dependent variables over the previous time step; (2) the absolute value of the maximum change in the dependent variables, averaged over the last NITAVG time steps; (3) the L_2 norm of the residual for each equation; (4) the average residual for each equation; or (5) the maximum residual for each equation. These parameters are defined in Section 4.1.6 of Volume 2.

The convergence criteria to be used and the level to be reached are set by the input parameters ICTEST and EPS. Each dependent variable or equation is checked separately, and convergence is declared when the specified level is reached for all of the variables or equations. The same criteria is used for each one, but different levels may be specified.

Subroutine CONV first computes ΔQ_{max} , the absolute value of the maximum change in each dependent variable over all the grid points for the most recent time step. These values are stored in CHGMAX(IVAR,1), where IVAR varies from 1 to NEQ, the number of dependent variables. If ICTEST = 2 (the so-called "moving average" convergence test), CHGMAX(IVAR,2) contains the maximum change for the previous time step, etc.

Then, depending on the value of ICTEST, the chosen convergence criteria is compared with the level to be reached for each dependent variable or equation, and a flag is set if the calculation is converged.

Remarks

1. For ICTEST = 1 or 2, the change in E_T is divided by $R/(\gamma_r - 1) + 1/2$. This is equivalent to dividing the dimensional value \bar{E}_T by

$$E_{T_r} = \frac{\rho_r \bar{R} T_r}{\gamma_r - 1} + \frac{\rho_r u_r^2}{2}$$

This makes the change in total energy the same order of magnitude as the other conservation variables.

2. For ICTEST = 1 or 2, the convergence test is based on (or includes) the change in dependent variables from time level n to $n + 1$. For ICTEST = 3, 4, or 5, convergence is based on the residual at time level n , not $n + 1$. This is because the residuals at time level $n + 1$ are not computed until the marching step from $n + 1$ to $n + 2$ is taken.
3. For cases run with artificial viscosity, the residuals are computed and printed both with and without the artificial viscosity terms. This may provide some estimate of the overall error in the solution introduced by the artificial viscosity. Convergence is determined by the residuals with the artificial viscosity terms included.
4. The Cray search routine ISAMAX is used in computing the absolute value of the maximum change in dependent variables.
5. The scratch array DUMMY, from the common block DUMMY1, is used to store the values of the change in dependent variables for use by ISAMAX.
6. A warning message is generated if an illegal convergence criteria is specified. ICTEST is reset to 3 (convergence based on the L_2 norm of the residual), and the calculation will continue.

Subroutine CUBIC (IDIR,T,G,NOLD,TINT,GINT)		
Called by	Calls	Purpose
PAK		Interpolation using Ferguson's parametric cubic.

Input

G	A two-dimensional array containing $NOLD1 \times NOLD2$ values of the function $g(t)$ to be interpolated.
IDIR	Direction flag; 1 if first subscript in G varies, 2 if second subscript varies.
I1, I2	Grid indices i and j , in the ξ and η directions.
NOLD	Number of values in direction IDIR in array G (i.e., NOLD1 or NOLD2.)
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
T	A one-dimensional array containing NOLD values of the independent variable t .
TINT	A one-dimensional array containing N1 or N2 (depending on IDIR) values of the independent variable $t = t_{int}$ at which interpolated values $g_{int} = g(t_{int})$ are desired.

Output

GINT	A one-dimensional array containing N1 or N2 (depending on IDIR) interpolated values $g_{int} = g(t_{int})$.
------	--

Description

Subroutine CUBIC performs interpolation using Ferguson's parametric cubic polynomial (Faux and Pratt, 1979). Given the function $g(t)$ and a value t_{int} , CUBIC computes $g_{int} = g(t_{int})$.

The function $g(t)$ is specified by the Fortran arrays G and T. For a general value t , let

$$t_f = \frac{t - t_u}{t_d - t_u}$$

where $t_u \leq t \leq t_d$. (I.e., t_u and t_d are the two elements of the array T that bracket t .)

Between t_u and t_d , assume g can be described by a cubic polynomial in t_f , as follows:

$$g = a_1 + a_2 t_f + a_3 t_f^2 + a_4 t_f^3$$

Differentiating,

$$g' = \frac{dg}{dt_f} = a_2 + 2a_3 t_f + 3a_4 t_f^2$$

Noting that $t_f = 0$ at $t = t_u$, and 1 at $t = t_d$, we get

$$\begin{aligned}
g_u &= a_1 \\
g'_u &= a_2 \\
g_d &= a_1 + a_2 + a_3 + a_4 \\
g'_d &= a_2 + 2a_3 + 3a_4
\end{aligned}$$

Solving for a_1 through a_4 ,

$$\begin{aligned}
a_1 &= g_u \\
a_2 &= g'_u \\
a_3 &= 3(g_d - g_u) - 2g'_u - g'_d \\
a_4 &= 2(g_u - g_d) + g'_u + g'_d
\end{aligned}$$

Plugging these into the cubic polynomial for f and rearranging,

$$\begin{aligned}
g &= g_u(1 - 3t_f^2 + 2t_f^3) + g_d(3t_f^2 - 2t_f^3) \\
&\quad + g'_u(t_f - 2t_f^2 + t_f^3) + g'_d(-t_f^2 + t_f^3)
\end{aligned}$$

This is the form of the equation used to compute g_{int} .

Remarks

1. At interior points in the array g , the derivatives g'_u and g'_d are computed using a second-order central difference formula. At the end points, second-order one-sided difference formulas are used.
2. The Fortran variable TINT is actually a one-dimensional array containing N_1 or N_2 input values of t_{int} . Similarly, GINT is a one-dimensional array containing N_1 or N_2 output values of g_{int} .
3. The Fortran array G that specifies the input values of $g(t)$ is actually a two-dimensional array. Within CUBIC, however, only one of the subscripts varies. The input flag IDIR specifies which one.

Subroutine EQSTAT (ICALL)		
Called by	Calls	Purpose
BVUP EXEC INITC MAIN		Use equation of state to compute pressure, temperature, and their derivatives with respect to the dependent variables.

Input

CP, CV	Specific heats c_p and c_v .
* HSTAG	Stagnation enthalpy h_T used with constant stagnation enthalpy option.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
ICALL	0 to get p and T , 1 to get derivatives of p and T with respect to dependent variables.
* IHSTAG	Flag for constant stagnation enthalpy option.
NPTS	Number of grid points in the sweep direction, N .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
RGAS	Gas constant R .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T .

Output

DPDRHO, DPDRU, DPDRV, DPDRW, DPDET	Derivatives $\partial p/\partial \rho$, $\partial p/\partial(\rho u)$, $\partial p/\partial(\rho v)$, $\partial p/\partial(\rho w)$, and $\partial p/\partial E_T$.
DTDRHO, DTDRU, DTDRV, DTDRW, DTDET	Derivatives $\partial T/\partial \rho$, $\partial T/\partial(\rho u)$, $\partial T/\partial(\rho v)$, $\partial T/\partial(\rho w)$, and $\partial T/\partial E_T$.
ET	Total energy (constant stagnation enthalpy option only.)
INEG	Flag for non-positive pressure and/or temperature; 0 if positive, 1 if non-positive.
P, T	Static pressure p and temperature T .

Description

Subroutine EQSTAT computes various quantities that depend on the form of the equation of state. It actually serves a dual purpose. First, it is called from subroutine INITC and from the MAIN program, with the input parameter ICALL = 0, to compute the static pressure p and temperature T from the initial or just-computed values of the dependent variables. If the constant stagnation enthalpy option is being used it also computes a value for the total energy E_T . And second, it is called from subroutines BVUP and EXEC, with ICALL = 1, to compute the derivatives of p and T with respect to the dependent variables.²⁵

The equation of state currently built into *Proteus* is for a perfect gas. The formulas used to compute p , T , and their derivatives with respect to the dependent variables are presented in Section 4.3 of Volume 1 for two-dimensional planar flow and in Section B.2.3 of Volume 1 for axisymmetric flow.

²⁵ These are needed for linearization of the governing equations. See Section 4.1 of Volume 1 for details.

Remarks

1. When used to compute p and T ($ICALL = 0$), this subroutine is called from outside any loops in the ξ or η directions. When used to compute $\partial p / \partial \rho$, etc., ($ICALL = 1$), it is called for each ADI sweep from inside a loop in the non-sweep direction.
2. When computing $\partial p / \partial \rho$, etc., this subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.

Subroutine EXEC		
Called by	Calls	Purpose
MAIN	ADI AVISC1 AVISC2 BCELM BCGEN BVUP COEFC COEFE COEFX COEFY COEFZ EQSTAT PERIOD RESID UPDATE	Manage solution of governing equations.

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_z .
* IAV2E, IAV4E, IAV2I	Flags for second-order explicit, fourth-order explicit, and second-order implicit artificial viscosity.
* IAXI	Flag for axisymmetric flow.
IBCELM	Flags for elimination of off-diagonal coefficient submatrices resulting from three-point boundary conditions in the ξ and η directions at either boundary; 0 if elimination is not necessary, 1 if it is.
* ICHECK	Convergence checking interval.
* IHSTAG	Flag for constant stagnation enthalpy option.
* ISWIRL	Flag for swirl in axisymmetric flow.
IT	Current time step number n .
ITBEG	The time level n at the beginning of a run.
* ITHIN	Flags for thin-layer option.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
NEQP	Dimensioning parameter specifying maximum number of coupled equations allowed.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
NTABC	Dimensioning parameter specifying total storage required for the coefficient submatrices A, B, and C.
NTS	Dimensioning parameter specifying total storage required for the source term subvector S.

* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
N1P, N2P	Parameters specifying the dimension sizes in the ξ and η directions.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .
Y	Radial coordinate r for axisymmetric flow.

Output

DEL	Computational grid spacing in sweep direction.
IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
ISWEEP	Current ADI sweep number.
IV	Index in the "vectorized" direction, i_v .
I1, I2	Grid indices i and j , in the ξ and η directions.
JI	The radius times the inverse Jacobian of the nonorthogonal grid transformation, rJ^{-1} (used in COEF routines for axisymmetric flow only.)
METX, METY, METT	Derivatives of sweep direction computational coordinate with respect to x , y (or r if axisymmetric), and t .
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
RAX	1 for two-dimensional planar flow, and the local radius r for axisymmetric flow.
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level $n + 1$.
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
TL	Static temperature T at time level n .

Description

Subroutine EXEC manages the solution of the governing equations. It is called by the MAIN program during each marching step from time level n to $n + 1$. The steps involved in EXEC are described below.

Preliminary Steps

1. If this is the first time step, temporarily set the thin-layer flags to zero.
2. Initialize the coefficient submatrices **A**, **B**, and **C**, and the source term subvector **S**, to zero.
3. If spatially periodic boundary conditions are being used in either direction, call PERIOD to add the appropriate extra line(s) of data.

First ADI sweep, ξ direction

4. Set various sweep-dependent parameters, as follows:

```

isweep = 1
istep  = 1
del     =  $\Delta\xi$ 
npts    =  $N_1$  or  $N_1 + 1$ 
nv      =  $N_2$  or  $N_2 + 1$ 

```

5. For axisymmetric flow, set $JI = r/J$ at all grid points.
6. Set metrics in sweep (ξ) direction at all grid points as follows:

$$\begin{aligned}\text{metx}(\text{i2}, \text{i1}) &= (\xi_x)_{i,j} \\ \text{metry}(\text{i2}, \text{i1}) &= (\xi_y)_{i,j} \text{ or } (\xi_r)_{i,j} \\ \text{mett}(\text{i2}, \text{i1}) &= (\xi_t)_{i,j}\end{aligned}$$

7. Begin loop in non-sweep (η) direction over interior points ($j = I2 = 2$ to $NPT2 - 1$).
8. For axisymmetric flow, set $RAX(I1) = r_{i,j}$ along the current η -line at all ξ grid points.
9. Call EQSTAT to get the derivatives of p and T with respect to ρ , ρu , etc., along the current η -line at all ξ grid points.
10. Call the COEF routines to compute the coefficients and source terms for the governing equations along the current η -line at all interior ξ grid points.
11. End of loop in non-sweep (η) direction.
12. For axisymmetric flow, reset $JI = 1/J$ at all grid points.
13. For non-spatially periodic boundary conditions in the ξ direction, begin loop in non-sweep (η) direction over interior points ($j = I2 = 2$ to $NPT2 - 1$).
14. Call EQSTAT to get the derivatives of p and T with respect to ρ , ρu , etc., along the current η -line at all ξ grid points.
15. Call BCGEN to compute the coefficients and source terms for the boundary condition equations at the end points ($i = I1 = 1$ and N_1) of the current η -line.
16. If three-point boundary conditions were used at either boundary, call BCELIM to eliminate the resulting off-diagonal coefficient submatrices.
17. End of loop in non-sweep (η) direction.
18. Every ICHECK time steps, call RESID to compute residuals at time level n without the artificial viscosity terms, and to update the convergence history file.
19. If artificial viscosity is being used, call AVISC1 or AVISC2 to add the appropriate terms to the coefficient submatrices and/or the source term subvectors at all interior grid points.
20. Every ICHECK time steps, if artificial viscosity is being used, call RESID to compute residuals at time level n with the artificial viscosity terms, and to update the convergence history file.
21. If spatially periodic boundary conditions are being used in the ξ direction, reset $NPTS = N_1$.
22. Call ADI to solve the system of difference equations.
23. Begin loop in non-sweep (η) direction over interior points ($j = I2 = 2$ to $NPT2 - 1$).
24. Call UPDATE to compute the primitive flow variables, Q^* , from the newly computed conservation variables in delta form, $\Delta \hat{Q}^*$, along the current η -line at all ξ grid points.
25. End of loop in non-sweep (η) direction.

Second ADI sweep, η direction

26. Set various sweep-dependent parameters, as follows:

$$\begin{aligned}\text{isweep} &= 2 \\ \text{istep} &= \text{nlp} \\ \text{del} &= \Delta \eta \\ \text{npts} &= N_2 \text{ or } N_2 + 1 \\ \text{nv} &= N_1 \text{ or } N_1 + 1\end{aligned}$$

27. For axisymmetric flow, set $JI = r/J$ at all grid points.

28. Set metrics in sweep (η) direction at all grid points as follows:

```
metx(i1,i2) = ( $\eta_x$ )i,j
metry(i1,i2) = ( $\eta_y$ )i,j or ( $\eta_r$ )i,j
mett(i1,i2) = ( $\eta_t$ )i,j
```

29. Begin loop in non-sweep (ξ) direction over interior points ($i = I1 = 2$ to $NPT1 - 1$).

30. For axisymmetric flow, set $RAX(I2) = r_{i,j}$ along the current ξ -line at all η grid points.

31. Call EQSTAT to get the derivatives of p and T with respect to ρ , ρu , etc., along the current ξ -line at all η grid points.

32. Call the COEF routines to compute the coefficients and source terms for the governing equations along the current ξ -line at all interior η grid points.

33. End of loop in non-sweep (ξ) direction.

34. For axisymmetric flow, reset $JI = 1/J$ at all grid points.

35. For non-spatially periodic boundary conditions in the η direction, begin loop in non-sweep (ξ) direction over interior points ($i = I1 = 2$ to $NPT1 - 1$).

36. Call EQSTAT to get the derivatives of p and T with respect to ρ , ρu , etc., along the current ξ -line at all η grid points.

37. Call BCGEN to compute the coefficients and source terms for the boundary condition equations at the end points ($j = I2 = 1$ and N_2) of the current ξ -line.

38. If three-point boundary conditions were used at either boundary, call BCELIM to eliminate the resulting off-diagonal coefficient submatrices.

39. End of loop in non-sweep (ξ) direction.

40. If implicit artificial viscosity is being used, call AVISC1 to add the appropriate terms to the coefficient submatrices at all interior grid points.

41. If spatially periodic boundary conditions are being used in the η direction, reset $NPTS = N_2$.

42. Call ADI to solve the system of difference equations.

43. Begin loop in non-sweep (ξ) direction over interior points ($i = I1 = 2$ to $NPT1 - 1$).

44. Call UPDATE to compute the primitive flow variables ρ^{n+1} , u^{n+1} , etc., from the newly computed conservation variables in delta form, $\Delta \hat{Q}^n$, along the current ξ -line at all η grid points.

45. End of loop in non-sweep (ξ) direction.

Finishing Steps

46. If this is the first time step, reset the thin-layer flags back to their input value.

47. Call BVUP to update the ξ boundary values, if necessary.

48. For all grid points, shift RHO and RHOL so that $RHO = \rho^{n+1}$ and $RHOL = \rho^n$. Similarly, shift the Fortran variables for u , v , w , and E_T . Finally, set $TL = T^n$.

Subroutine EXECT		
Called by	Calls	Purpose
TURBCH	BLK2 BLK2P COEFS1 COEFS2 PERIOD UPDTKE	Manage solution of the k - ε equations.

Input

A	Coefficient submatrix A .
* CMUR	Constant C_μ , in formula for C_μ .
* CTHREE	Constant C_3 in formula for C_μ .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
N1P, N2P	Parameters specifying the dimension sizes in the ξ and η directions.
RHO	Static density ρ at time level n .
S	Source term subvector S .
YPLUSD	Nondimensional distance y^+ from the nearest solid wall.

Output

E, EL	Turbulent dissipation rate ε at time levels $n + 1$ and n .
ISWEEP	Current ADI sweep number.
KE, KEL	Turbulent kinetic energy k at time levels $n + 1$ and n .
MUT, MUTL	Turbulent viscosity μ_t at time levels $n + 1$ and n .
NPTS	Number of grid points in the sweep direction, N .
NV	Number of grid points in the "vectorized" direction, N_v .
S	Computed solution subvector $\Delta \hat{W}$.

Description

Subroutine EXECT manages the solution of the k - ε equations. It is called by subroutine TURBCH, NTKE times per mean flow iteration. The steps involved in EXECT are described below.

Preliminary Steps

1. If spatially periodic boundary conditions are being used in either direction, call PERIOD to add the appropriate extra line(s) of data.

First ADI sweep, ξ direction

2. Set various sweep-dependent parameters.
3. Call COEFS1 to compute the coefficients and source terms for the k - ε equations.
4. Solve the system of difference equations by calling BLK2 for non-periodic boundary conditions, or BLK2P for periodic boundary conditions in the ξ direction.

Second ADI sweep, η direction

5. Set various sweep-dependent parameters.
6. Swap indices in the subvector S. The submatrix A is used as a temporary scratch array for this operation.
7. Call COEFS2 to compute the coefficients and source terms for the k - ε equations.
8. Solve the system of difference equations by calling BLK2 for non-periodic boundary conditions, or BLK2P for periodic boundary conditions in the η direction.

Finishing Steps

9. For all grid points, set $KEL = k^n$ and $EL = \varepsilon^n$.
10. Call UPDTKE to compute the primitive flow variables k^{n+1} and ε^{n+1} from $\Delta \hat{W}^n$, the newly computed conservation variables in delta form.
11. Compute the turbulent viscosity at each grid point, storing μ_t^{n+1} and μ_t^n in MUT and MUTL, respectively.

Subroutine FILTER (A,B,C,S,NVD,NPTSD)		
Called by	Calls	Purpose
BLK3 BLK4 BLK5	BLKOUT ISAMAX ISRCHQ	Rearrange rows of the boundary condition coefficient submatrices and the source term subvector to eliminate any zeroes on the diagonal.

Input

A, B, C	Coefficient submatrices A, B, and C before rearrangement.
* IDEBUG	Debug flags.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ISWEEP	Current ADI sweep number.
IT	Current time step number n .
IV	Index in the "vectorized" direction, i_v .
NEQ	Number of coupled equations being solved, N_{eq} .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NPTS	Number of grid points in the sweep direction, N .
NVD, NPTSD	Leading two dimensions for the arrays A, B, C, and S.
S	Source term subvector S before rearrangement.

Output

A, B, C	Coefficient submatrices A, B, and C after rearrangement.
S	Source term subvector S after rearrangement.

Description

Subroutine FILTER rearranges rows of the coefficient block submatrices and the source term subvector, at the two boundaries in the ADI sweep direction, in an attempt to eliminate any zero values on the diagonal of the submatrix B. These zero values may occur when mean flow boundary conditions are specified using the JBC and/or IBC input parameters, depending on the initial conditions and the order of the boundary conditions.

For instance, if the specified initial conditions are zero velocity and constant flow properties everywhere in the flow field, the perfect gas equation of state yields:

$$\begin{aligned}
 E_T &= \rho c_v T \\
 p &= (\gamma - 1) E_T \\
 \frac{\partial p}{\partial \rho} &= \frac{\partial p}{\partial(\rho u)} = \frac{\partial p}{\partial(\rho v)} = 0 \\
 \frac{\partial p}{\partial E_T} &= \gamma - 1
 \end{aligned}$$

$$\frac{\partial T}{\partial \rho} = -\frac{E_T}{c_v \rho^2}$$

$$\frac{\partial T}{\partial(\rho u)} = \frac{\partial T}{\partial(\rho v)} = 0$$

$$\frac{\partial T}{\partial E_T} = \frac{1}{c_v \rho}$$

If, in addition, the boundary conditions at a given boundary are, in order, specified pressure $p=f$, no-slip x - and y -velocity $u=0$ and $v=0$, and specified temperature $T=f$, then the linearization of the boundary conditions leads to the following **B** coefficient submatrix for that boundary:

$$\mathbf{B} = \begin{bmatrix} 0 & 0 & 0 & J(\gamma - 1) \\ 0 & J/\rho & 0 & 0 \\ 0 & 0 & J/\rho & 0 \\ -JE_T/c_v \rho^2 & 0 & 0 & J/c_v \rho \end{bmatrix}$$

The zero on the diagonal will lead to a divide-by-zero error in subroutine BLK4, even though this is not a singular matrix.

Subroutine FILTER tries to fix this problem. In this example, it finds a zero at element B_{11} , searches column 1 for the largest element in absolute value (in this case $-JE_T/c_v \rho^2$), and adds that row to the row with the zero on the diagonal. Of course, the corresponding rows of **A**, **C**, and **S** must also be added together. The new **B** submatrix would be:

$$\mathbf{B} = \begin{bmatrix} -JE_T/c_v \rho^2 & 0 & 0 & J(\gamma - 1) + J/c_v \rho \\ 0 & J/\rho & 0 & 0 \\ 0 & 0 & J/\rho & 0 \\ -JE_T/c_v \rho^2 & 0 & 0 & J/c_v \rho \end{bmatrix}$$

Remarks

1. If a column with a zero on the diagonal has no other elements greater than 10^{-10} , then it is assumed that the matrix **B** is singular, which means the specified boundary conditions are not independent of one another. An error message is printed and the calculation is stopped.
2. It's probably sufficient to only call this subroutine for the first time step. After the first step, the chances of u and v both being exactly zero at the same interior grid point are slim. Nevertheless, in the current version of *Proteus*, FILTER is called at every time step.
3. The Cray search routine ISAMAX is used in finding the largest element in any column corresponding to a zero on the matrix diagonal. The Cray search routine ISRCHEQ is used in determining the grid locations for debug printout.
4. This subroutine generates the output for the IDEBUG(4) option.

Subroutine FTEMP		
Called by	Calls	Purpose
INITC MAIN		Compute auxiliary variables that are functions of temperature.

Input

CCP1, CCP2, CCP3, CCP4	Constants in formula for specific heat.
CK1, CK2	Constants in formula for laminar thermal conductivity coefficient.
CMU1, CMU2	Constants in formula for laminar viscosity coefficient.
* GAMR	Reference ratio of specific heats, γ_r .
IGAM	Flag for constant or variable c_p , c_v , and γ ; 0 if they are to be computed as functions of temperature, 1 if they are to be treated as constant.
* ILAMV	Flag for computation of laminar viscosity and thermal conductivity.
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
RGAS	Gas constant R .
T	Static temperature T .
* TR, UR, MUR, KTR	Reference temperature T_r , velocity u_r , viscosity μ_r , and thermal conductivity k_r .

Output

CP, CV	Specific heats c_p and c_v .
MU, LA, KT	Laminar coefficient of viscosity μ_l , laminar second coefficient of viscosity λ_l , and laminar coefficient of thermal conductivity k_l .

Description

Subroutine FTEMP computes the auxiliary variables μ_l , λ_l , k_l , c_p , and c_v . For the laminar viscosities μ_l and λ_l , and the laminar thermal conductivity k_l , there are two options currently available.

If the input parameter ILAMV = 0 (the default), FTEMP sets the nondimensional values as:

$$\begin{aligned}\mu_l &= 1 \\ \lambda_l &= -2/3 \\ k_l &= 1\end{aligned}$$

Thus, with this option, the laminar viscosity and thermal conductivity are held constant at their reference values. These reference values may be specified by the user, or computed from the reference temperature. The laminar second coefficient of viscosity λ_l is set equal to $-2\mu_l/3$.

If ILAMV = 1, μ_l and k_l are computed as functions of temperature using Sutherland's formula (White, 1974). The formula for the laminar viscosity coefficient μ_l is

$$\mu_l = \frac{\bar{\mu}_l}{\mu_r} = \frac{\mu'_r}{\mu_r} \frac{T_r + C_{\mu 2}}{\bar{T} + C_{\mu 2}} \left(\frac{\bar{T}}{T_r} \right)^{3/2}$$

where the overbar indicates a dimensional value, and μ'_r is the laminar viscosity coefficient at $\bar{T} = T_r$, given by

$$\mu'_r = C_{\mu 1} \frac{T_r^{3/2}}{T_r + C_{\mu 2}}$$

Depending on the namelist input values of MUR and RER, μ'_r may or may not be equal to μ_r . These formulas are valid for air for temperatures from 300 to 3420 °R (167 to 1900 K). The value of the constants $C_{\mu 1}$ and $C_{\mu 2}$ depend on whether reference values are being specified by the user in English units (IUNITS = 0) or SI units (IUNITS = 1). The values are presented in Table 4-1. The laminar second coefficient of viscosity λ_l is set equal to $-2\mu_l/3$. The formula for the laminar thermal conductivity coefficient k_l is

$$k_l = \frac{\bar{k}_l}{k_r} = \frac{k'_r}{k_r} \frac{T_r + C_{k 2}}{\bar{T} + C_{k 2}} \left(\frac{\bar{T}}{T_r} \right)^{3/2}$$

where the overbar indicates a dimensional value, and k'_r is the laminar thermal conductivity coefficient at $\bar{T} = T_r$, given by

$$k'_r = C_{k 1} \frac{T_r^{3/2}}{T_r + C_{k 2}}$$

Depending on the namelist input values of KTR and PRLR, k'_r may or may not be equal to k_r . These formulas are valid for air for temperatures from 300 to 1800 °R (167 to 1000 K). The value of the constants $C_{k 1}$ and $C_{k 2}$ depend on whether reference values are being specified by the user in English units (IUNITS = 0) or SI units (IUNITS = 1). The values are presented in Table 4-1.

There are also two options available for the specific heat coefficients c_p and c_v . If the flag IGAM = 1, a value of the specific heat ratio γ has been specified by the user. In this case c_p and c_v are treated as constants, and computed from

$$c_v = \frac{R}{\gamma - 1}$$

$$c_p = c_v + R$$

If IGAM = 0, the user did not specify a value of γ . In this case, the specific heat coefficient c_p is computed as a function of temperature from the empirical formula of Hesse and Mumford (1964), and c_v is computed from that value assuming a thermally perfect gas. The ratio $\gamma = c_p/c_v$ will then vary with temperature. The equations for c_p and c_v are:

$$c_p = \bar{c}_p \frac{T_r}{u_r^2} = \frac{T_r}{u_r^2} (C_{c_p 1} - C_{c_p 2} \bar{T}^{-1/2} - C_{c_p 3} \bar{T} + C_{c_p 4} \bar{T}^2)$$

$$c_v = c_p - R$$

This formula is valid for air for temperatures from 540 to 9000 °R (300 to 5000 K). The values of the constants $C_{c_p 1}$ through $C_{c_p 4}$ are presented in Table 4-1.

TABLE 4-1. - EMPIRICAL CONSTANTS FOR μ_l , k_l , AND c_p

CONSTANT	ENGLISH UNITS	SI UNITS
$C_{\mu 1}$	7.3035×10^{-7}	1.4582×10^{-6}
$C_{\mu 2}$	198.6	110.3
$C_{k 1}$	7.4907×10^{-3}	1.8641×10^{-3}
$C_{k 2}$	350.0	194.4
$C_{cp 1}$	8.53×10^3	1.4264×10^3
$C_{cp 2}$	3.12×10^4	3.8888×10^3
$C_{cp 3}$	2.065×10^6	1.9184×10^5
$C_{cp 4}$	7.83×10^8	4.0413×10^7

Remarks

1. The formulas used with the ILAMV = 1 option are for air. For other fluids, different formulas should be used to compute μ_l , λ_l , and k_l . These could easily be programmed as additional ILAMV options. Or, if the flow being computed is such that μ_l and k_l may be considered constant, simply set ILAMV = 0 and read in the appropriate values for μ_r and k_r . Note, however, that the ILAMV = 0 option still sets $\lambda_l = -2\mu_l/3$.
2. The formula used to compute c_p , when a value of γ is not specified by the user, is for air. For other gases, a different formula should be programmed. Or, if c_p and c_v may be considered constant, a value of γ should be read in.
3. An error message is generated and execution is stopped if an illegal value is specified for ILAMV.

Subroutine GEOM		
Called by	Calls	Purpose
MAIN	METS PAK	Manage computation of grid and metric parameters.

Input

- * IPACK Flags for grid packing option.
- * NGEOM Flag for type of computational coordinates.
- * NGRID Unit number for input mesh file.
- * NOUT Unit number for standard output.
- * N1, N2 Number of grid points N_1 and N_2 , in the ξ and η directions.
- N1P, N2P Parameters specifying the dimension sizes in the ξ and η directions.
- * RMIN, RMAX Minimum and maximum r' -coordinates for polar grid.
- * THMIN, THMAX Minimum and maximum θ' -coordinates for polar grid.
- * XMIN, XMAX Minimum and maximum x -coordinates for Cartesian grid.
- * YMIN, YMAX Minimum and maximum y -coordinates for Cartesian grid.

Output

- DXI, DETA Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
- X, Y Cartesian coordinates x and y , or cylindrical coordinates x and r .

Description

Subroutine GEOM manages the computation of the grid and metric parameters. There are currently three coordinate system options built into *Proteus*, as follows:

<u>NGEOM</u>	<u>Computational Coordinates</u>
1	Cartesian (x - y)
2	Polar (r' - θ')
10	Read from separate file.

Subroutine GEOM first computes the grid spacing in computational space in the ξ and η directions as $\Delta\xi = 1/(N_1 - 1)$ and $\Delta\eta = 1/(N_2 - 1)$. Note that grid points in computational space are always evenly distributed along the (ξ - η) coordinate lines.

Cartesian (x - y) Coordinates ($NGEOM = 1$)

For the Cartesian coordinate option, an evenly spaced set of physical Cartesian (x - y) coordinates are related to the computational (ξ - η) coordinates by

$$x = x_{min} + (x_{max} - x_{min})\xi$$

$$y = y_{min} + (y_{max} - y_{min})\eta$$

These equations also apply to axisymmetric flow, with y representing the radius r . If grid packing is used, subroutine PAK is called to redistribute these points according to the packing parameters specified by the

user, and to interpolate to get the new physical Cartesian (x - y) coordinates in the computational mesh. Subroutine METS is then called to numerically compute the grid transformation metrics and Jacobian.

Polar (r' - θ') Coordinates (NGEOM = 2)

For the polar coordinate option, an evenly spaced set of physical polar (r' - θ') coordinates are related to the computational (ξ - η) coordinates by

$$\begin{aligned}\theta' &= \theta'_{min} + (\theta'_{max} - \theta'_{min})\xi \\ r' &= r'_{min} + (r'_{max} - r'_{min})\eta\end{aligned}$$

The Cartesian (x - y) coordinates are simply given by

$$\begin{aligned}x &= r' \cos \theta' \\ y &= r' \sin \theta'\end{aligned}$$

The above equations also could be used in axisymmetric flow, with y representing the radius r . As in the NGEOM = 1 option, if grid packing is used, subroutine PAK is called to redistribute these points according to the packing parameters specified by the user, and to interpolate to get the new physical Cartesian (x - y) coordinates in the computational mesh. Subroutine METS is then called to numerically compute the grid transformation metrics and Jacobian.

Coordinates Read From Separate File (NGEOM = 10)

The third option for specifying the computational coordinate system is to read it from a separate file, as described in Section 3.2 of Volume 2. The computational (ξ - η) coordinate system is determined by a set of $N_{G1} \times N_{G2}$ points whose physical Cartesian (x - y) coordinates are specified. Here N_{G1} , and N_{G2} are the number of points in the ξ and η directions used to specify the computational coordinate system. Note that they do not have to be equal to N_1 and N_2 , the number of points in the computational mesh used for the finite-difference method.²⁶ Note also that the points do not have to be equally distributed in physical space along the ξ and η coordinate lines.

If grid packing is being used, subroutine PAK is called to distribute $N_1 \times N_2$ computational mesh points in physical space according to the packing parameters SQ specified by the user, and to interpolate among the $N_{G1} \times N_{G2}$ points in the input computational coordinate system to get the new physical Cartesian coordinates of the points in the computational mesh.

If grid packing is not being used, but N_{G1} and N_{G2} are not equal to N_1 and N_2 respectively, then subroutine PAK is still called. In this case, however, PAK distributes the $N_1 \times N_2$ computational mesh points evenly in physical space and then interpolates among the $N_{G1} \times N_{G2}$ points in the input computational coordinate system to get the new physical Cartesian coordinates of the points in the computational mesh.

In either case, subroutine METS is then called to numerically compute the grid transformation metrics and Jacobian.

Remarks

1. There may be some confusion between the axisymmetric flow option and the polar coordinate system option, or between the axisymmetric radius r and the polar coordinate r' . They are not the same thing. The governing flow equations were originally developed by writing them in Cartesian (x - y) coordinates, then transforming them into generalized (ξ - η) coordinates. Therefore, any computational coordinate system that is used, including the polar coordinate system, must be related to the original Cartesian system through the transformation metrics and Jacobian. The parameters r' and θ' are used only to initially define the coordinates in the NGEOM = 2 option. Now, if the (x - y) coordinates, no matter how they are obtained, are rotated about the Cartesian x axis, the result is a cylindrical coordinate co-

²⁶ The distinction between the computational coordinate system and the computational mesh is described in Section 2.2 of Volume 2.

ordinate system with y representing the radius r . Thus, the axisymmetric flow option can be used with any of the coordinate system options. The polar coordinate option would be useful, for instance, for flow over a sphere.

2. An error message is generated and execution is stopped if an illegal coordinate system option is specified.
3. With the `NGEOM = 10` option, an error message is generated and execution is stopped if N_{G1} and/or N_{G2} are greater than the dimensioning parameters `N1P` and/or `N2P`.

Subroutine INIT		
Called by	Calls	Purpose
INITC		Get user-defined initial flow field.

Input

- * ICVARS Flag specifying which variables are being supplied as initial conditions by subroutine INIT.
- NIN Unit number for namelist input.
- * NOUT Unit number for standard output.
- * N1, N2 Number of grid points N_1 and N_2 , in the ξ and η directions.

Output

- P, T, U, V, W Initial flow field values of static pressure p , static temperature T , and velocities u , v , and w .

Description

Subroutine INIT supplies the user-defined initial flow field. In general, this subroutine will be tailored to the problem being solved, and supplied by the user. Details on the variables to be supplied by INIT are presented in Section 5.1 of Volume 2.

A default version of INIT is supplied with *Proteus* that specifies uniform flow with constant properties everywhere in the flow field. The above list of input and output Fortran variables are for the default version of INIT. The default version assumes ICVARS = 2 (the default value), and reads values of p_0 , u_0 , v_0 , w_0 , and T_0 from namelist IC. The defaults for these parameters are 1.0, 0.0, 0.0, 0.0, and 1.0, respectively, resulting in an initial flow field with $\bar{p} = p_r$, $u = v = w = 0$, and $\bar{T} = T_r$.

Remarks

1. If a value for ICVARS other than 2 is set in the input, a warning message is generated and ICVARS is reset to 2.
2. Subroutine INIT is a convenient place to specify point-by-point boundary condition types and values. It's often easier to do this using Fortran coding rather than entering each value into the namelist input file.

Subroutine INITC		
Called by	Calls	Purpose
MAIN	EQSTAT FTEMP INIT KEINIT REST TURBBL YPLUSN	Set up consistent initial conditions based on data from INIT.

Input

* CMUR	Constant C_{μ_r} in formula for C_μ .
* CTHREE	Constant C_3 in formula for C_μ .
* GAMR	Reference ratio of specific heats, γ_r .
GC	Proportionality factor g_c in Newton's second law.
* HSTAG	Stagnation enthalpy h_T used with constant stagnation enthalpy option.
* ICVARS	Flag specifying which variables are being supplied as initial conditions by subroutine INIT.
* IHSTAG	Flag for constant stagnation enthalpy option.
* IREST	Flag for reading restart file.
ITBEG	The time level n at the beginning of a run.
* ITURB	Flag for turbulent flow option.
* KBC1, KBC2	Boundary types for the ξ and η directions.
LWSET	Flags specifying how wall locations are to be determined for the turbulence model; 0 if wall locations are to be found automatically by searching for boundary points where the velocity is zero, 1 if input using the LWALL parameters, 2 if input using the IWALL parameters.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
PR	Reference pressure p_r .
RGAS	Gas constant R .
* RHOR, UR	Reference density ρ_r and velocity u_r .
INITIAL FLOW FIELD	From the user-supplied or default version of subroutine INIT. The combination of variables supplied by INIT is specified by ICVARS. See Section 5.0 of Volume 2 for details.

Output

LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries, if not set in input.
MUT, MUTL	Turbulent viscosity μ_t at time levels n and $n - 1$.
RHO, U, V, W, ET	Initial flow field values of static density ρ , velocities u , v , and w , and total energy E_T at time level n .

RHOL, UL, VL, WL, ETL

Initial flow field values of static density ρ , velocities u , v , and w , and total energy E_T at time level $n - 1$.

TL

Static temperature T at time level $n - 1$.

Description

Subroutine INTC sets up consistent initial flow field conditions based on the data supplied by subroutine INIT. For restart cases, subroutine REST is called to read the computational mesh and the initial flow field. Otherwise, the data supplied by INIT are used to obtain the density ρ , the velocities u , v , and w , and the temperature T .²⁷ It then calls FTEMP to compute the laminar viscosity coefficients μ_l and λ_l , the laminar thermal conductivity coefficient k_l , and the specific heat coefficients c_p and c_v . EQSTAT is called next to compute the pressure p and to recompute the temperature T .²⁸ For turbulent flow, the appropriate subroutines are called to compute the effective viscosity and thermal conductivity coefficients using the turbulence model specified by the user. And finally, for non-restart cases, the values of the dependent variables at time level $n - 1$ are set equal to the values at level 1.

The flag ICVARS is used to specify which combination of variables are being supplied by INIT. The calculation of ρ , u , v , w , and T is described below for the different values of ICVARS. In all of the equations below, the specific heats are defined by

$$c_v = \frac{R}{\gamma_r - 1}$$

$$c_p = R + c_v$$

where γ_r is either specified by the user or computed from the reference temperature T_r .

ICVARS = 1

With this option, the density ρ , the momentum components ρu , ρv , and ρw , and if IHSTAG = 0 the total energy E_T , are supplied by INIT. Thus, the velocity components are simply

$$u = \frac{\rho u}{\rho}$$

$$v = \frac{\rho v}{\rho}$$

$$w = \frac{\rho w}{\rho}$$

If the energy equation is being solved (IHSTAG = 0), the temperature is computed from

$$T = \frac{1}{c_v} \left[\frac{E_T}{\rho} - \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

If the energy equation is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), the temperature is computed from

$$T = \frac{1}{c_p} \left[h_T - \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

²⁷ The calculation of T at this point may be approximate. See Remark 1.

²⁸ See Remark 1.

ICVARS = 2

With this option, the pressure p and the velocities u , v , and w are supplied by INIT. If the energy equation is being solved (IHSTAG = 0), the temperature T is also supplied by INIT. If it is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), the temperature is computed from

$$T = \frac{1}{c_p} \left[h_T - \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

The density is then given by

$$\rho = \frac{p}{RT}$$

and the total energy is

$$E_T = \rho \left[c_v T + \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

ICVARS = 3

With this option, the density ρ and the velocities u , v , and w are supplied by INIT. If the energy equation is being solved (IHSTAG = 0), the temperature T is also supplied by INIT. If it is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), the temperature is computed from

$$T = \frac{1}{c_p} \left[h_T - \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

The total energy is then

$$E_T = \rho \left[c_v T + \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

ICVARS = 4

With this option, the pressure p and the velocities u , v , and w are supplied by INIT. If the energy equation is being solved (IHSTAG = 0), the density ρ is also supplied by INIT. If it is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), this option is the same as the ICVARS = 2 option. If the energy equation is being solved, then, the temperature is

$$T = \frac{p}{\rho R}$$

The total energy is then

$$E_T = \rho \left[c_v T + \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

ICVARS = 5

With this option, the static pressure coefficient c_p and the velocities u , v , and w are supplied by INIT. If the energy equation is being solved (IHSTAG = 0), the temperature T is also supplied by INIT. If it is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), the temperature is computed from

$$T = \frac{1}{c_p} \left[h_T - \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

The pressure coefficient is defined by

$$c_p = \frac{(\bar{p} - p_r)g_c}{\rho_r u_r^2 / 2}$$

The nondimensionalized pressure $p = \bar{p}g_c/\rho_r u_r^2$ is thus

$$p = \frac{c_p}{2} + \frac{p_r g_c}{\rho_r u_r^2}$$

or, since $p_r = \rho_r \bar{R} T_r / g_c$ and the nondimensionalized gas constant $R = \bar{R} T_r / u_r^2$,

$$p = \frac{c_p}{2} + R$$

The density is then

$$\rho = \frac{p}{RT}$$

and the total energy is

$$E_T = \rho \left[c_v T + \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

ICVARS = 6

With this option, the pressure p , Mach number M , and flow angles α_v and α_w are supplied by INIT. If the energy equation is being solved (IHSTAG = 0), the temperature T is also supplied by INIT. If it is being eliminated by assuming constant stagnation enthalpy (IHSTAG = 1), the temperature is computed from

$$T = T_T \left(1 + \frac{\gamma_r - 1}{2} M^2 \right)^{-1}$$

where $T_T = h_T / c_p$. The density is

$$\rho = \frac{p}{RT}$$

The flow angles are defined by $\alpha_v = \tan^{-1}(v/u)$ and $\alpha_w = \tan^{-1}(w/u)$. The Mach number is defined by

$$M = \left(\frac{u^2 + v^2 + w^2}{\gamma_r R T} \right)^{1/2}$$

Solving for u ,

$$u = M \left[\frac{\gamma_r R T}{1 + (v/u)^2 + (w/u)^2} \right]^{1/2}$$

where $(v/u)^2 = \tan^2 \alpha_v$ and $(w/u)^2 = \tan^2 \alpha_w$. The remaining velocities are simply

$$v = u \tan \alpha_v$$

$$w = u \tan \alpha_w$$

The total energy is

$$E_T = \rho \left[c_v T + \frac{1}{2} (u^2 + v^2 + w^2) \right]$$

Remarks

1. If T is not supplied by INIT, it must be computed from the equation of state. The equation of state contains a specific heat coefficient (either c_p or c_v , depending on whether the stagnation enthalpy is assumed constant or not.) The first time T is computed in INITC, a constant value of specific heat is used, consistent with the reference temperature T_r . If the user specified constant specific heat (i.e., a value for γ_r was read in), this is not a problem. However, if the temperature-dependent specific heat option is being used (i.e., a value for γ_r was not read in), the equation of state and the empirical equation for specific heat are coupled. For this reason T is recomputed in EQSTAT after the specific heats are computed in FTEMP. Ideally, this coupling would be handled by iteration between FTEMP and EQSTAT. This is not currently done in *Proteus*, however.
2. For options in which the pressure p is specified (ICVARS = 2, 4, and 6), the value supplied by INIT is redefined as follows:

$$p = p_r \frac{p_r g_c}{\rho_r u_r^2}$$

This is necessary because input and output values of p are nondimensionalized by the reference pressure $p_r = \rho_r \bar{R} T_r$, while internal to the code itself p is nondimensionalized by the normalizing pressure $p_n = \rho_r u_r^2$. See Section 3.1.1 of Volume 2 for a discussion of the distinction between reference and normalizing conditions.

3. With the ICVARS = 6 option, the initial velocity u will be limited to non-negative values.
4. If non-positive pressures or temperatures were computed in EQSTAT, the Fortran variable INEG will be positive. An error message will be printed, including a table showing the location of the non-positive values. The calculation will stop in INITC.
5. An error message is generated and execution is stopped if an illegal value is specified for ICVARS.
6. An error message is generated and execution is stopped if the value of ITURB does not correspond to an existing turbulence model.

Subroutine INPUT		
Called by	Calls	Purpose
MAIN	ISAMAX	Read and print input, perform various initializations.

Input

NIN	Unit number for namelist input.
NTP	Dimensioning parameter specifying the maximum number of entries in the table of time-dependent boundary condition values.
NTSEQP	Dimensioning parameter specifying the maximum number of time step sequences for the time step sequencing option.
N1P, N2P	Parameters specifying the dimension sizes in the ξ and η directions.

Output

CKMIN	Constant $(C_{Kleb})_{min}$ in the Klebanoff intermittency factor.
GAMR	Reference ratio of specific heats, γ_r .
HSTAG, HSTAGR	Dimensionless and dimensional stagnation enthalpy h_T for the constant stagnation enthalpy option.
IGAM	Flag for constant or variable c_p , c_v , and γ ; 0 if they are to be computed as functions of temperature, 1 if they are to be treated as constant.
IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
ITDBC	Flag for time-dependent boundary conditions; 0 if all boundary conditions are steady, 1 if any general unsteady boundary conditions are used, 2 if only steady and time-periodic boundary conditions are used.
LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries.
LWSET	Flags specifying how wall locations are to be determined for the turbulence model; 0 if wall locations are to be found automatically by searching for boundary points where the velocity is zero, 1 if input using the LWALL parameters, 2 if input using the IWALL parameters.
MACHR	Reference Mach number M_r .
MUR, KTR	Reference viscosity coefficient μ_r and thermal conductivity coefficient k_r .
NEQ	Number of coupled equations being solved, N_{eq} .
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
NRW, NET	Array indices associated with the dependent variables ρw and E_T .
NZM, NEN	Array indices associated with the swirl momentum and energy equations.
PR	Reference pressure p_r .
PRLR	Reference laminar Prandtl number Pr_l .
RER, PRR	Reference Reynolds number Re_r and Prandtl number Pr_r .

RGAS	Gas constant R .
UR	Reference velocity u_r .

Description

Subroutine INPUT performs various input and initialization functions. It first reads the title and namelist input from the standard input file. Namelist RSTRT is read first, followed by namelist IO. If IUNITS = 1, indicating reference conditions will be specified in SI units, various default values and constants are redefined to be consistent with SI units. The remaining namelists are then read.

Next, the flags controlling the time step cycling and the convergence testing method are redefined, if necessary, to be consistent with each other. The number of equations being solved, and the array indices corresponding to the energy and swirl momentum equations, are then determined based on the values of IHSTAG and ISWIRL. A flag is set if time-dependent boundary conditions are being used. If the thin-layer option is being used, the flags ITXI and ITETA used in the Baldwin-Lomax turbulence model are automatically set equal to values consistent with the thin-layer approximation. The LWSET flags, which specify how wall locations are to be determined for the turbulence model, are defined based on the default and input values of the LWALL and IWALL parameters. If the user did not specify a value for $(C_{kleb})_{min}$, it is set to the default value, which depends on the turbulence model being used.

Next, if frequency of printout in the ξ and η directions is being set by the input arrays IPRT1 and IPRT2, the corresponding grid indices are stored in arrays IPRT1A and IPRT2A. The total number of printout locations in each direction is also determined.

A header is then written to the standard output file, followed by the input namelists. Note that, for variables not specified by the user in the input namelists, the values in this printout will be the default values.

Various checks are made for inconsistent or invalid input, and appropriate error or warning messages are written. These are described in Section 7.0 of Volume 2.

Next, any reference or normalizing conditions not already defined are calculated. The reference and normalizing conditions are then written to the standard output file, with the appropriate units. See Section 3.1.1 of Volume 2 for a discussion of the distinction between reference and normalizing conditions.

Remarks

1. The Cray search routine ISAMAX is used in the input consistency check to determine whether any implicit artificial viscosity coefficients are non-zero.

Function ISAMAX (N,V,INC)		
Called by	Calls	Purpose
BLOUT1 BLOUT2 CONV FILTER INPUT RESID TIMSTP		Find the first index corresponding to the largest absolute value of the elements of a Fortran vector.

Input

N	Number of elements to process in the vector (i.e., N = vector length if INC = 1, N = (vector length)/2 if INC = 2, etc.).
V	Vector to be searched.
INC	Skip distance between elements of V. For contiguous elements, INC = 1.

Output

ISAMAX	First index corresponding to the largest absolute value of the elements of V that were searched.
--------	--

Description

Function ISAMAX finds the first index corresponding to the largest absolute value of the elements of a vector. For a one-dimensional vector, the use of ISAMAX is straightforward. For example,

```
imax = isamax(np,v,1)
```

sets IMAX equal to the index I corresponding to the maximum value of V(I) for I = 1 to NP.

A starting location can be specified, as in

```
imax = 4 + isamax(np-4,v(5),1)
```

which sets IMAX equal to the index I corresponding to the maximum value of V(I) for I = 5 to NP.

Multi-dimensional arrays can be used by taking advantage of the way Fortran arrays are stored in memory, and specifying the proper vector length and skip distance. For instance, if A is an array dimensioned NDIM1 by NDIM2, then

```
imax = isamax(ndim1*ndim2,a,1)
```

sets IMAX equal to the one-dimensional index corresponding to the maximum value of A(I,J) for all I and J. The maximum value of A can then be referenced as A(IMAX,1).

One dimension at a time can also be searched. For example,

```
imax = isamax(ndim1,a(1,5),1)
```

sets IMAX equal to the index I corresponding to the maximum value of A(I,5) for I varying from 1 to NDIM1. Similarly, by specifying a skip increment,

```
jmax = isamax(ndim2,a(5,j),ndim1)
```

sets JMAX equal to the index J corresponding to the maximum value of A(5,J) for J varying from 1 to NDIM2.

Remarks

1. ISAMAX is a Cray search routine (Cray Research, Inc., 1989b).

Function ISAMIN (N,V,INC)		
Called by	Calls	Purpose
BLOUT1 BLOUT2		Find the first index corresponding to the smallest absolute value of the elements of a Fortran vector.

Input

N	Number of elements to process in the vector (i.e., N = vector length if INC = 1, N = (vector length)/2 if INC = 2, etc.).
V	Vector to be searched.
INC	Skip distance between elements of V. For contiguous elements, INC = 1.

Output

ISAMIN	First index corresponding to the smallest absolute value of the elements of V that were searched.
--------	---

Description

Function ISAMIN finds the first index corresponding to the smallest absolute value of the elements of a vector. It is used in exactly the same way as ISAMAX.

Remarks

1. ISAMIN is a Cray search routine (Cray Research, Inc., 1989b).

Function ISRCHEQ (N,V,INC,VALUE)		
Called by	Calls	Purpose
BCGEN BLIN1 BLIN2 BLOUT1 BLOUT2 FILTER		Find the first index in a vector whose element is equal to a specified value.

Input

N	Number of elements to process in the vector (i.e., N = vector length if INC = 1, N = (vector length)/2 if INC = 2, etc.).
V	Vector to be searched.
INC	Skip distance between elements of V. For contiguous elements, INC = 1.
VALUE	Value to be searched for in the vector V.

Output

ISRCHEQ	First index, of the elements of V that were searched, whose element is equal to the value V. If the value V is not found, the returned value will be N + 1.
---------	---

Description

Function ISRCHEQ finds the first index in a vector whose element is equal to a specified value. For a one-dimensional vector, the use of ISRCHEQ is straightforward. For example,

```
ival = isrcheq(np,v,1,val)
```

searches V(I), for I = 1 to NP, for the value VAL, and sets IVAL equal to the first index I for which V(I) = VAL. If the value VAL is not found, IVAL will be equal to NP + 1.

A starting location can be specified, as in

```
ival = 4 + isrcheq(np-4,v(5),1,val)
```

which searches V(I), for I = 5 to NP, for the value VAL.

Multi-dimensional arrays can be used by taking advantage of the way Fortran arrays are stored in memory, and specifying the proper vector length and skip distance. For instance, if A is an array dimensioned NDIM1 by NDIM2, then

```
ival = isrcheq(ndim1*ndim2,a,1,val)
```

searches A(I,J), for all I and J, for the value VAL, and sets IVAL equal to the corresponding one-dimensional index. The desired indices in A can then be recovered from

```
i = mod(ival-1,ndim1) + 1
j = (ival-1)/ndim1 + 1
```

One dimension at a time can also be searched. For example,

```
ival = isrcheq(ndim1,a(1,5),1,val)
```

searches A(I,5), for I = 1 to NDIM1, for the value VAL. Similarly, by specifying a skip increment,

```
jval = isrcheq(ndim2,a(5,j),ndim1,val)
```

searches A(5,J), for J = 1 to NDIM2, for the value VAL.

Remarks

1. ISRCHEQ is a Cray search routine (Cray Research, Inc., 1989b).

Subroutine KEINIT		
Called by	Calls	Purpose
INITC	PRODC TURBBL YPLUSN	Get user-defined initial conditions for k and ε .

Input

* CMUR	Constant C_{μ_r} in formula for C_μ .
* CTHREE	Constant C_3 in formula for C_μ .
DUMMY	Distance to the nearest solid wall.
MUT	Turbulent viscosity μ_t at time level n .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
VORT	Production rate of turbulent kinetic energy.
YPLUSD	Nondimensional distance y^+ from the nearest solid wall.

Output

E, EL	Turbulent dissipation rate ε at time levels n and $n - 1$.
KE, KEL	Turbulent kinetic energy k at time levels n and $n - 1$.
MUTL	Turbulent viscosity μ_t at time level $n - 1$.

Description

Subroutine KEINIT supplies the user-defined initial values of the turbulent kinetic energy k and the turbulent dissipation rate ε . In general, this subroutine will be tailored to the problem being solved, and supplied by user. Details on the variables to be supplied by KEINIT are presented in Section 5.1 of Volume 2.

A default version of KEINIT is supplied with *Proteus* that computes the initial values of k and ε using the assumption of local equilibrium (dissipation equals production.) The above list of input and output Fortran variables are for the default version of KEINIT.

The steps involved in the default version of KEINIT are described below.

1. Initialize k and ε to zero.
2. Call TURBBL to compute turbulent viscosity values and to locate solid walls in the computational domain.
3. Call YPLUSN to compute y^+ and the minimum distance to the nearest solid wall.
4. Call PRODC to compute the production rate of turbulent kinetic energy.
5. Compute k and ε using

$$C_\mu = C_{\mu_r} (1 - e^{C_3 y^+})$$

$$\varepsilon = \left| \frac{P_k}{Re_r \rho} \right|$$

$$k = \sqrt{\frac{\mu_t \varepsilon}{C_{\mu} \rho}}$$

6. Set the values of k , ε , and μ_t at time level $n - 1$ equal to their values at time level n .

Remarks

1. The scratch array DUMMY, from the common block DUMMY1, is used to store the values of the minimum distance to the nearest wall. The array is filled in subroutine YPLUSN.
2. The Fortran array VORT, from the common block TURB1, is used to store the values of the production rate of turbulent kinetic energy. The array is filled in subroutine PRODCET.

Program MAIN		
Called by	Calls	Purpose
	BCSET CONV EQSTAT EXEC FTEMP GEOM INITC INPUT OUTPUT OUTW PLOT PRTHST REST TBC TIMSTP TREMAIN TURBBL TURBCH	Manage overall solution.

Input

None.

Output

IT	Current time step number n .
ITEND	Final time step number.
ITSEQ	Current time step sequence number.
TAU	Current time value τ .

Description

The MAIN program is used to manage the overall solution. The steps involved are described below.

Preliminary Steps

1. Call INPUT to read and print the input, and perform various initialization procedures.
2. Unless this is a restart case, call GEOM to get the computational coordinates and metric data.
3. Call INITC to get the initial flow field.
4. Call BCSET to set various boundary condition parameters and flags, and to print the input boundary condition types and values.
5. Initialize the plot file,²⁹ and, if requested by the user, write the initial or restart flow field into the plot file.
6. If requested by the user, print the initial or restart flow field.

²⁹ The initialization procedure depends on the type of plot file being written. See the description of subroutine PLOT.

7. Compute NTSUM, the maximum total number of marching steps to be taken, and ITEND, the corresponding final index on the time marching loop. Set the initial values of ITSEQ, the time step sequence number, and ITSWCH, the time index for switching to the next sequence, both to zero.

Time marching loop

8. Begin the time marching loop. The loop index IT corresponds to the known time level n . Each iteration of the loop thus corresponds to a step from time level n to $n + 1$.
9. If at the end of a time step sequence, update ITSEQ, the time step sequence number, and ITSWCH, the time index for switching to the next sequence.
10. For the first time step, and every IDTMOD'th step thereafter, call TIMSTP to compute the new time step $\Delta\tau$. For every time step update the time value τ .
11. If time-dependent boundary conditions are being used, call TBC to set the boundary condition values.
12. Call EXEC to solve the equations.
13. Call EQSTAT to compute the pressure p and temperature T from the equation of state. If either is non-positive, indicating a non-physical solution, skip forward to step 17.
14. Call FTEMP to compute the laminar viscosities μ_i and λ_i , the laminar thermal conductivity k_i , and the specific heats c_p and c_v .
15. For turbulent flow, call the appropriate subroutines to compute the effective viscosity and thermal conductivity coefficients using the turbulence model specified by the user.
16. Every ICHECK time levels, call CONV to check for convergence.
17. Call TREMAIN to find out how much CPU time remains.
18. If requested by the user, or if the calculation is converged, or if non-positive pressures or temperatures were computed, or if the job is near the CPU time limit, print the flow field at time level $n + 1$.
19. If requested by the user, or if the calculation is converged, or if non-positive pressures or temperatures were computed, or if the job is near the CPU time limit, write the flow field at time level $n + 1$ into the plot file.
20. If non-positive pressures or temperatures were computed, write an error message showing the location of the non-positive values and skip forward to step 25, ending the calculation.
21. If the calculation is converged, print a message and skip forward to step 24, ending the calculation.
22. If the job is near the CPU time limit, print a message and skip forward to step 24, ending the calculation.
23. End of time marching loop. Print a message indicating the calculation did not converge.

Final Steps

24. If requested by the user, call REST to write the restart file.
25. If first-order time differencing and steady boundary conditions were used, call PRTHST to print the convergence history.

Remarks

1. The starting index for the time marching loop is ITBEG. For a non-restart case ITBEG = 1, and thus the initial starting flow field is at time level 1. For a restart case ITBEG = n , where n is the time level stored in the restart file, and thus the starting flow field is the previously computed flow field at time level n .
2. The ending index for the time marching loop is ITEND = ITBEG + NTSUM - 1, where NTSUM is the total number of time steps to be taken. For a non-restart case, then, the time marches from level

1 to level $1 + \text{NTSUM}$. For a restart case, the time marches from level ITBEG to level $\text{ITBEG} + \text{NTSUM}$.

3. The logic involving NTSUM, ITSEQ, and ITSWCH is used to implement the time step sequencing option. This allows one CFL number or time increment to be used for a specified number of steps, followed by another CFL number or time increment for another specified number of steps, etc.³⁰ If this option is not used, NTSUM is simply equal to NTIME(1) and ITSEQ is always 1.
4. An error message is generated and execution is stopped if the value of ITURB does not correspond to an existing turbulence model.
5. Although the calculation will stop if p or $T \leq 0$, as noted above in step 20, the standard output and plot file will include the time level with the non-positive values, if that is consistent with the IPRT and IPLT input parameters in namelist IO. The restart file will not be written.

³⁰ See Section 3.1.9 of Volume 2 for details on how to invoke the time step sequencing option.

Subroutine METS		
Called by	Calls	Purpose
GEOM REST	OUTPUT	Compute metrics of nonorthogonal grid transformation.

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
* IDEBUG	Debug flags.
* IVOUT	Flags specifying variables to be printed.
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

ETAX, ETAY, ETAT	Metric coefficients η_x, η_y (or η_r if axisymmetric), and η_t .
IVOUT	Flags specifying variables to be printed (temporarily redefined for debug output of metrics.)
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
XIX, XIY, XIT	Metric coefficients ξ_x, ξ_y (or ξ_r if axisymmetric), and ξ_t .

Description

Subroutine METS computes the metric coefficients and the Jacobian for the generalized nonorthogonal coordinate transformation. The metric coefficients are defined in terms of the known (x,y) coordinates of the computational mesh as:

$$\xi_x = Jy_\eta$$

$$\xi_y = -Jx_\eta$$

$$\eta_x = -Jy_\xi$$

$$\eta_y = Jx_\xi$$

$$\xi_t = -x_t\xi_x - y_t\xi_y$$

$$\eta_t = -x_t\eta_x - y_t\eta_y$$

where J is the Jacobian of the transformation, given by

$$J = \frac{1}{J^{-1}} = (x_\xi y_\eta - x_\eta y_\xi)^{-1}$$

The derivatives of x and y with respect to the computational coordinates are computed numerically using the same difference formulas as used for the governing equations. At interior points the centered difference formula presented in Section 5.0 of Volume 1 is used. At boundaries three-point one-sided differencing is used. For ξ -derivatives at the $\xi = 0$ and $\xi = 1$ boundaries,

$$\frac{\partial f}{\partial \xi} \simeq \pm \frac{-3f_w + 4f_{w \pm 1} - f_{w \pm 2}}{2\Delta \xi}$$

where w represents the ξ -index at the boundary (i.e., either 1 or N_1). Where a \pm sign appears, the $+$ sign is used at the $\xi = 0$ boundary, and the $-$ sign is used at the $\xi = 1$ boundary. An analogous formula is used for η -derivatives at the $\eta = 0$ and $\eta = 1$ boundaries.

Remarks

1. Since the current version of *Proteus* is limited to meshes that do not vary with time, the derivatives x_t and y_t are set equal to zero.
2. This subroutine generates the output for the IDEBUG(7) option.
3. An error message is generated and execution is stopped if the grid transformation Jacobian J changes sign or equals zero. This indicates that the computational mesh contains crossed or coincident grid lines. The error message is followed by a printout of the Cartesian coordinates, the Jacobian, and the metric coefficients.

Subroutine OUTPUT (LEVEL)		
Called by	Calls	Purpose
MAIN METS	PRTOUT VORTEX	Manage printing of output.

Input

CP, CV	Specific heats c_p and c_v .
DTAU	Time step $\Delta\tau$.
DUMMY	A two-dimensional scratch array dimensioned (N1P,N2P).
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
E, KE	Turbulent dissipation rate ε and kinetic energy k .
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* GAMR	Reference ratio of specific heats, γ_r .
GC	Proportionality factor g_c in Newton's second law.
* IAXI	Flag for axisymmetric flow.
* ISWIRL	Flag for swirl in axisymmetric flow.
* IVOUT	Flags specifying variables to be printed.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
LEVEL	Time level being printed.
LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries.
* MACHR	Reference Mach number M_r .
MU, LA, KT	Effective coefficient of viscosity μ , effective second coefficient of viscosity λ , and effective coefficient of thermal conductivity k .
MUT	Turbulent viscosity coefficient μ_t .
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
P, T	Static pressure p and temperature T .
PR	Reference pressure p_r .
PRR	Reference Prandtl number Pr_r .
* PRT	Turbulent Prandtl number Pr_t .
RGAS	Gas constant R .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T .
* RHOR, TR, UR	Reference density ρ_r , temperature T_r , and velocity u_r .
TAU	Time value τ .
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .

Output

ATITLE	A 20-character title for variable being printed.
DUMMY	A two-dimensional array containing the variable to be printed.

Description

Subroutine OUTPUT manages the printing of the standard output. The variables available for printing are listed and defined in Table 3-3 of Volume 2. The user-specified array IVOUT controls which variables are printed.

Each variable to be printed is stored, in turn, in the scratch array DUMMY, from the common block DUMMY1. The title printed with the variable is stored in the character array ATITLE. Subroutine PRTOUT is then called to execute the actual write statements.

Remarks

1. A warning message is printed if a non-existent output variable is requested. The printout will continue with the next requested output variable.
2. For output options 30, 31, 34, and 35, involving the pressure p , the value stored internally in the *Proteus* code is redefined as follows:

$$p = p \frac{\rho_r u_r^2}{p_r g_c}$$

This is necessary because input and output values of p are nondimensionalized by the reference pressure $p_r = \rho_r \bar{R} T_r$, while internal to the code itself p is nondimensionalized by the normalizing pressure $p_n = \rho_r u_r^2$. See Section 3.1.1 of Volume 2 for a discussion of the distinction between reference and normalizing conditions.

3. The definitions of k_t and k_r (IVOUT = 92 and 102) assume a constant turbulent Prandtl number is being specified in namelist TURB. If the input value of PRT ≤ 0 , indicating the use of a variable turbulent Prandtl number, the printed values of k_t and k_r will be incorrect.

Subroutine OUTW (LEVEL)		
Called by	Calls	Purpose
MAIN		Compute and print parameters at boundaries.

Input

CP	Specific heat c_p .
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY	Metric coefficients η_x and η_y (or η , if axisymmetric.)
GC	Proportionality factor g_c in Newton's second law.
* IWOUT1, IWOUT2	Flags specifying for which boundaries parameters are to be printed.
LEVEL	Time level being printed.
MU, KT	Effective coefficients of viscosity μ , and thermal conductivity k .
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
P, T	Static pressure p and temperature T .
PR	Reference pressure p_r .
PRR	Reference Prandtl number Pr_r .
* RER	Reference Reynolds number Re_r .
* RHOR, UR	Reference density ρ_r , and velocity u_r .
U, V, W	Velocities u , v , and w .
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ , if axisymmetric.)

Output

None.

Description

Subroutine OUTW computes and prints various parameters along the computational boundaries. The variables available for printing are listed and defined in Table 3-3 of Volume 2. The user-specified arrays IWOUT1 and IWOUT2 specify at which boundaries parameters are printed, and whether normal derivatives are to be computed using two-point or three-point one-sided differencing.

The parameters printed are the Cartesian coordinates x and y , the static pressure p , the skin friction coefficient c_f , the shear stress τ_w , the static temperature T , the heat transfer coefficient h , the heat flux q_w , and the Stanton number St . Note that some of these are meaningful only if the boundary is a solid wall.

The skin friction coefficient is defined as

$$c_f = \frac{\bar{\mu} \frac{\partial \bar{V}_t}{\partial \bar{n}}}{\frac{1}{2} \rho_r u_r^2} = \frac{2}{Re_r} \mu \frac{\partial V_t}{\partial n}$$

where the overbar denotes a dimensional quantity. In this equation $\partial V_t / \partial n$ represents the normal derivative of the tangential velocity, with the normal vector \vec{n} directed into the flow field.

For a ξ boundary, the tangential velocity for non-swirl cases is simply

$$V_t = V_\eta$$

where V_η is the velocity in the η direction. For axisymmetric cases with swirl, the tangential velocity on a ξ boundary is computed as

$$V_t = \sqrt{V_\eta^2 + w^2}$$

where w is the swirl velocity. From the description of subroutine BCVDIR,

$$V_\eta = \frac{1}{m} (-\xi_y u + \xi_x v)$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

Using the equations in Section 6.4 of Volume 1, $\partial V_t / \partial n$ for a ξ boundary is thus computed as

$$\frac{\partial V_t}{\partial n} = \pm \frac{1}{m} \left[\frac{\partial V_t}{\partial \xi} (\xi_x^2 + \xi_y^2) + \frac{\partial V_t}{\partial \eta} (\xi_x \eta_x + \xi_y \eta_y) \right]$$

where the + sign is used at the $\xi = 0$ boundary, and the - sign is used at the $\xi = 1$ boundary.

For an η boundary, the tangential velocity for non-swirl cases is

$$V_t = V_\xi$$

and for axisymmetric cases with swirl, it is computed as

$$V_t = \sqrt{V_\xi^2 + w^2}$$

The ξ velocity is given by

$$V_\xi = \frac{1}{m} (\eta_y u + \eta_x v)$$

where

$$m = \sqrt{\eta_x^2 + \eta_y^2}$$

Thus, for an η boundary,

$$\frac{\partial V_t}{\partial n} = \pm \frac{1}{m} \left[\frac{\partial V_t}{\partial \xi} (\xi_x \eta_x + \xi_y \eta_y) + \frac{\partial V_t}{\partial \eta} (\eta_x^2 + \eta_y^2) \right]$$

The shear stress τ_w is defined as

$$\tau_w = \mu \frac{\partial V_t}{\partial n}$$

τ_w is thus nondimensionalized by $\mu_\infty u_\infty / L_\infty$.

The heat flux q_w is defined as

$$q_w = -k \frac{\partial T}{\partial n}$$

where $\partial T/\partial n$ represents the normal derivative of the temperature. For a ξ boundary,

$$\frac{\partial T}{\partial n} = \pm \frac{1}{m} \left[\frac{\partial T}{\partial \xi} (\xi_x^2 + \xi_y^2) + \frac{\partial T}{\partial \eta} (\xi_x \eta_x + \xi_y \eta_y) \right]$$

where

$$m = \sqrt{\xi_x^2 + \xi_y^2}$$

For an η boundary,

$$\frac{\partial T}{\partial n} = \pm \frac{1}{m} \left[\frac{\partial T}{\partial \eta} (\eta_x^2 + \eta_y^2) + \frac{\partial T}{\partial \xi} (\xi_x \eta_x + \xi_y \eta_y) \right]$$

where

$$m = \sqrt{\eta_x^2 + \eta_y^2}$$

q_w is thus nondimensionalized by $k_r T_r / L_r$.

The heat transfer coefficient h is defined as

$$h = \frac{q_w}{T - 1} = \frac{-k \frac{\partial T}{\partial n}}{T - 1}$$

This is the nondimensional form of the equation

$$\bar{h} = \frac{\bar{q}_w}{\bar{T} - T_r} = \frac{-\bar{k} \frac{\partial \bar{T}}{\partial \bar{n}}}{\bar{T} - T_r}$$

h is thus nondimensionalized by k_r / L_r .

The Stanton number St is defined as

$$St = \frac{\bar{h}}{\rho_r u_r \bar{C}_p} = \frac{h}{c_p} \frac{1}{Re_r Pr_r}$$

Subroutine PAK (IDIR,NOLD1,NOLD2)		
Called by	Calls	Purpose
GEOM	CUBIC ROBTS	Manage packing and/or interpolation of grid points.

Input

IDIR	Direction flag; 1 if grid points are being redistributed in the ξ direction, 2 if in the η direction.
* IPACK	Flags for grid packing option.
NOLD1, NOLD2	Number of grid points in the ξ and η directions in the original grid.
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions in the new grid.
* SQ	An array specifying the location and amount of packing.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r , in the old grid.

Output

X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r , in the new grid.
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Description

Subroutine PAK manages the redistribution of the user-specified points in the computational coordinate system. It is called whenever grid packing is used. It is also called when interpolation is necessary because the computational coordinates are specified by reading them from a separate file (the NGEOM = 10 option in subroutine GEOM), and the number of points in the file is different from the number of points to be used in the calculation. PAK is called once for each direction in which points are being redistributed.

The steps involved in subroutine PAK are described below. For clarity, this discussion assumes IDIR = 1 (i.e., we are redistributing points in the ξ direction.) An exactly analogous procedure is used for IDIR = 2.

1. Set NNEW and NOLD equal to the index limits in the ξ direction for the new and old grids. Also set NOPP equal to the index limit in the η direction for the old grid.
2. Get $(a_p)_i$, the normalized physical arc length along a coordinate line in the ξ direction, from the beginning of the line to each grid point in the new grid. The normalizing distance is the total arc length of the line, and thus these arc lengths apply to any coordinate line in the ξ direction. If the points are not being packed in the ξ direction, but only interpolated, then

$$(a_p)_i = \frac{i-1}{NNEW-1}$$

for $i = 1$ to NNEW. In the new grid, the points will thus be evenly distributed in physical space along each coordinate line in the ξ direction. If the grid points are being packed in the ξ direction, subroutine ROBTS is called to compute $(a_p)_i$ from the packing parameters specified by the user.

3. Begin loop from IOPP = 1 to NOPP. This loop thus runs over the points in the η direction in the old grid. We will be redistributing points in the ξ direction for each η value in the old grid.

4. Get $(a_{UP})_i$, the normalized physical arc length along a coordinate line in the ξ direction, from the beginning of the line to each grid point in the old grid. These values are found by first computing the non-normalized arc lengths, as follows:

$$(a_{UP})_1 = 0$$

$$(a_{UP})_i = (a_{UP})_{i-1} + \sqrt{(x_{i,j} - x_{i-1,j})^2 + (y_{i,j} - y_{i-1,j})^2}$$

for $i = 2$ to NOLD1. These values are normalized by setting

$$(a_{UP})_i = \frac{(a_{UP})_i}{(a_{UP})_{\text{NOLD1}}}$$

for $i = 1$ to NOLD1. To eliminate any problems with roundoff error, $(a_{UP})_{\text{NOLD1}}$ is explicitly set equal to 1.

5. Given x and a_{UP} for the old grid, and a_P for the new grid, call CUBIC to interpolate for x in the new grid. Similarly interpolate for y .
6. Redefine the Fortran variables X and Y as the x and y coordinates in the new grid.
7. End of loop over the points in the η direction in the old grid.

Remarks

1. In the Fortran code, the comments sometimes refer to the "packing" direction. This terminology actually means the direction in which grid points are being redistributed, even if they are not being packed but only interpolated. Similarly, references to the "packed" and "unpacked" grid actually mean the new and old grids.
2. An error message is generated and execution is stopped if an invalid grid packing option is requested.

Subroutine PERIOD		
Called by	Calls	Purpose
EXEC EXECT		Define extra line of data for use in computing coefficients for spatially periodic boundary conditions.

Input

CP, CV	Specific heats c_p and c_v at time level n .
E, EL	Turbulent dissipation rate ϵ at time levels n and $n - 1$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_z .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions; 0 for non-periodic, 1 for periodic.
KE, KEL	Turbulent kinetic energy k at time levels n and $n - 1$.
MU, LA, KT	Effective coefficient of viscosity μ , effective second coefficient of viscosity λ , and effective coefficient of thermal conductivity k .
MUT, MUTL	Turbulent viscosity μ_t at time levels n and $n - 1$.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
P, T	Static pressure p and temperature T at time level n .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T from previous ADI sweep.
TL	Static temperature T from previous ADI sweep.
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_z .
Y	Radial coordinate r for axisymmetric flow.

Output

All of the flow and metric-related input parameters listed above, at $i = N_1 + 1$ for periodic boundary conditions in the ξ direction, and at $j = N_2 + 1$ for periodic boundary conditions in the η direction.

Description

Subroutine PERIOD adds, in effect, an additional set of points at $i = N_1 + 1$ for periodic boundary conditions in the ξ direction, and at $j = N_2 + 1$ for periodic boundary conditions in the η direction. This allows us to use central differencing in the periodic direction, at $i = N_1$ and/or $j = N_2$, computing the coefficient submatrices and source term subvector in the same way as at the interior points.³¹

For periodic boundary conditions in the ξ direction, the extra points are added by setting

³¹ See Section 7.2.2 of Volume 1 for details on the solution procedure for spatially periodic boundary conditions.

$$f_{N_1 + 1, j} = f_{2, j}$$

where $j = 1$ to N_2 , and f represents one of the flow variables or metrics. Similarly, extra points are added at $(i, N_2 + 1)$ for periodic boundary conditions in the η direction.

Subroutine PLOT (LEVEL)		
Called by	Calls	Purpose
MAIN		Write files for post-processing by CONTOUR or PLOT3D plotting programs.

Input

CP, CV	Specific heats c_p and c_v .
ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric).
* GAMR	Reference ratio of specific heats, γ_r .
GC	Proportionality factor g_c in Newton's second law.
* IPLOT	Flag specifying type of plot file to be written.
LEVEL	Time level to be written into the file (0 for initialization, and -1 to read the scratch file and write XYZ and Q files with the IPLOT = -3 option).
* LR, UR, RHOR, TR	Reference length L_r , velocity u_r , density ρ_r , and temperature T_r .
* MACHR	Reference Mach number M_r .
* NOUT	Unit number for standard output.
* NPLOT	Unit number for writing CONTOUR file, or PLOT3D Q file.
* NPLOTX	Unit number for writing PLOT3D XYZ file.
* NSCR1	Unit number for scratch file.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
P, T	Static pressure p and temperature T .
PR	Reference pressure p_r .
* RER	Reference Reynolds number Re_r .
* RG	Dimensional gas constant \bar{R} .
RGAS	Dimensionless gas constant R .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T .
TAU	Current time value τ .
* TITLE	Case title.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ_r if axisymmetric).

Output

None.

Description

Subroutine PLOT writes a file or files, commonly called plot files, for post-processing by the CONTOUR or PLOT3D plotting programs. The type of files written is controlled by the user-specified parameter IPLOT. The format and contents of the different types of plot files are described in detail in Section 4.2 of Volume 2. They are therefore described only briefly here.

CONTOUR Plot File (IPLOT = ± 1)

If IPLOT = 1, a CONTOUR plot file is written with the title and reference conditions included at each time level. The value of n is written into the header for each time level, but τ , the time itself, is not written into the file. No initialization step is necessary.

If IPLOT = - 1, a CONTOUR plot file is also written, but the title and reference conditions are written only at the beginning of the file. In addition the time $\tau_{i,j}$ is written into the file at each time level. In this case the initialization step consists of writing the title and reference conditions at the beginning of the file.

PLOT3D/WHOLE Plot Files (IPLOT = 2)

If IPLOT = 2, XYZ and Q files are written in PLOT3D/WHOLE format. The XYZ file is written only during the initialization step. The Q file is written at each time level requested by the user. The Q file will thus consist of multiple sets of data, each containing the computed results at a single time level. The time $\tau_{i,j}$ is written into the header for each set of data in the Q file. Since *Proteus* 2-D is two-dimensional, N3, the number of points in the z direction in the XYZ and Q files, is set equal to 1.

PLOT3D/PLANES Plot Files (IPLOT = 3)

If IPLOT = 3, XYZ and Q files are written in PLOT3D/PLANES format. Since *Proteus* 2-D is two-dimensional, N3, the number of points in the z direction in the XYZ and Q files, is set equal to 1. This makes the XYZ and Q files identical to those created using the IPLOT = 2 option.

PLOT3D/PLANES Plot Files (IPLOT = - 3)

The files created with this option are similar to those created with the IPLOT = 3 option, except the time $\tau_{i,j}$ is written into the z slot in the XYZ file, and the number of points in the " z " direction is set equal to the number of time levels in the XYZ and Q files.

However, because the calculation may converge or become non-physical, the number of time levels that end up being written into the files is not known until the end of the *Proteus* run. Therefore, as the calculation proceeds the results are actually written into a scratch file. N3, the counter for the number of time levels, is set equal to zero in the initialization step and updated each time a time level is added to the scratch file. At the end of the *Proteus* run the scratch file is read and the XYZ and Q files are written.

PLOT2D Plot Files (IPLOT = 4)

If IPLOT = 4, XYZ and Q files are written in PLOT3D's 2D format. The XYZ file is written only during the initialization step. The Q file is written at each time level requested by the user. The Q file will thus consist of multiple sets of data, each containing the computed results at a single time level. The time $\tau_{i,j}$ is written into the header for each set of data in the Q file.

Remarks

1. For the CONTOUR plot file, the IPLOT = - 1 option is the better one to use. The IPLOT = 1 option is included only to be consistent with the various PLOT3D options.
2. In defining the pressure to be written into the CONTOUR plot file, the value stored internally in the *Proteus* code is redefined as follows:

$$p = p \frac{\rho_r u_r^2}{p_r g_c}$$

This is necessary because input and output values of p are nondimensionalized by the reference pressure $p_r = \rho_r \bar{R} T_r$, while internal to the code itself p is nondimensionalized by the normalizing pressure $p_n = \rho_r u_r^2$. See Section 3.1.1 of Volume 2 for a discussion of the distinction between reference and normalizing conditions.

3. The current version of PLOT3D does not work for multiple time levels, although future versions might. Thus the IPLOT = 2, 3, and 4 options, while containing multiple time levels, cannot easily be used to create plots showing the time development of the flow. You can, however, fake it out using the IPLOT = -3 option. With this option, plots can be generated at different time levels by plotting at different PLOT3D "z" stations.
4. Note that the time $\tau_{1,1}$ written into the Q file header with the IPLOT = 2, 3, and 4 options is the time at the point $\xi = \eta = 0$. If the input variable IDTAU = 5 or 6, τ will vary in space and therefore $\tau_{i,j} \neq \tau_{1,1}$.
5. To save storage, the common variable AMAT1, which is normally used for the subdiagonal submatrix of coefficients in the block tridiagonal system of equations, is equivalenced to the local three-dimensional variable Q used to store the Q variables that are written into the PLOT3D Q file.
6. PLOT3D assumes that velocity is nondimensionalized by the reference speed of sound $a_r = (\gamma_r \bar{R} T_r)^{1/2}$, and that energy is nondimensionalized by $\rho_r a_r^2$. In *Proteus* these variables are nondimensionalized by u_r and $\rho_r u_r^2$. That is why the reference Mach number M_r appears in the definitions of Q(.,2) through Q(.,5).
7. An error message is generated and execution is stopped if an illegal plot file option is requested.

Subroutine PRODC		
Called by	Calls	Purpose
KEINIT TURBCH		Compute production term for the k - ϵ turbulence model.

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric).
* IAXI	Flag for axisymmetric flow.
MUT	Turbulent viscosity μ_t at time level n .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
* RER	Reference Reynolds number Re_r .
U, V, W	Velocities u , v , and w at time level n .
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ_r if axisymmetric).
Y	Radial coordinate r for axisymmetric flow.

Output

PONE, PTWO	Parts 1 and 2 of the production rate of turbulent kinetic energy.
VORT	Production rate of turbulent kinetic energy.

Description

Subroutine PRODC computes the turbulent kinetic energy production rate using

$$P_k = \frac{\mu_t}{Re_r} P_1 - \frac{2}{3} \rho k P_2$$

where, for 2-D planar flow,

$$P_1 = 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 \right] - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2 + \left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2$$

$$P_2 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}$$

and for axisymmetric flow,

$$P_1 = 2 \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial r} \right)^2 + \left(\frac{v}{r} \right)^2 \right] - \frac{2}{3} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{v}{r} \right)^2 + \left(\frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right)^2$$

$$+ \left(\frac{\partial w}{\partial x} \right)^2 + \left[r \frac{\partial}{\partial r} \left(\frac{w}{r} \right) \right]^2$$

$$P_2 = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial r} + \frac{v}{r}$$

To evaluate the spatial derivatives, the centered difference formulas presented in Section 5.0 of Volume 1 are used at interior points, and second-order one-sided difference formulas are used at boundary points.

Remarks

1. To save storage space, this subroutine uses the Fortran variable VORT to store the turbulent kinetic energy production rate. Care must be taken when this subroutine is used together with subroutine VORTEX.

Subroutine PRTHST		
Called by	Calls	Purpose
MAIN		Print convergence history.

Input

- * ICHECK Convergence checking interval.
- * IREST Flag for restart file; 0 for no restart file, 1 to write a restart file, 2 to read and write a restart file.
- IT Last computed time step number n .
- ITBEG The time level n at the beginning of a run.
- NC, NXM, NYM, NZM, NEN Array indices associated with the continuity, x -momentum, y -momentum (or r -momentum if axisymmetric), swirl momentum, and energy equations.
- NEQ Number of coupled equations being solved, N_{eq} .
- * NHIST Unit number for convergence history file.
- * NHMAX Maximum number of time levels allowed in the printout of the convergence history file (not counting the first two, which are always printed.)
- * NOUT Unit number for standard output.

Output

None.

Description

Subroutine PRTHST prints the convergence history as part of the standard output. The information is obtained from the unformatted convergence history file written in subroutine RESID. The parameters printed are described in Section 4.1.6 of Volume 2, and the unformatted convergence history file is described in Section 4.3 of Volume 2. To avoid undesirably long tables, the convergence parameters are printed at an interval that limits the printout to NHMAX time levels. As described in Section 4.1.6 of Volume 2, however, they are always printed at the first two time levels.

Subroutine PRTOUT (ATITLE,LEVEL,AVAR)		
Called by	Calls	Purpose
OUTPUT		Print output.

Input

ATITLE	A 20-character title for variable being printed.
AVAR	A two-dimensional array containing the variable to be printed.
DTAU	Time step $\Delta\tau$.
* IDTAU	Flag for time step selection method.
* IPRT1A, IPRT2A	Indices for printout in the ξ and η directions.
LEVEL	Time level to be printed.
* LR, UR	Reference length L_r and velocity u_r .
* NOUT	Unit number for standard output.
NPRT1, NPRT2	Total number of indices for printout in the ξ and η directions.
TAU	Current time value τ .

Output

None.

Description

Subroutine PRTOUT performs the actual printing of the standard output file. It prints the variable AVAR, with the title ATITLE. The output is printed in columns running in the η direction. The rows run in the ξ direction. If the results at every grid point are printed, there will be a total of N_1 columns, each with N_2 rows. The columns are grouped in super-rows of up to 10 columns each.

The steps involved are as follows:

1. Set the total number of columns, and rows per super-row.
2. Redefine AVAR, the input array containing the variable to be printed, including only the elements requested.
3. Determine the number of super-rows. If NCOL is not exactly divisible by 10, the last super-row will have less than 10 columns.
4. Print the title for the variable. If the time step is constant in space, the dimensional time t and time step Δt are printed with the title.
5. Begin loop over the number of super-rows.
6. Set NC1 and NC2 equal to the number of the first and last column in this super-row. (I.e., for the first super-row NC1 and NC2 will be 1 and 10, for the second they will be 11 and 20, etc. For the last super-row, NC2 will be NCOL.)
7. Print the heading for the super-row, labeling each column with the proper ξ index.
8. Print the super-row itself, labeling each row with the proper η index.
9. End of loop over the number of super-rows.

Subroutine RESID (IAVR,S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC	ISAMAX SASUM SNRM2	Compute residuals and write convergence history file.

Input

CHGAVG	Maximum change in absolute value of the dependent variables, averaged over the last NITAVG time steps, ΔQ_{avg} .
CHGMAX	Maximum change in absolute value of the dependent variables over previous time step (or NITAVG - 1 time steps if ICTEST = 2), ΔQ_{max} .
DTAU	Time step $\Delta \tau$.
DUMMY	A two-dimensional scratch array.
* EPS	Convergence level to be reached, ϵ .
IAVR	Flag specifying whether residual is computed without or with the artificial viscosity terms; 1 for without, 2 for with.
* IAV2E, IAV4E	Flags for second- and fourth-order explicit artificial viscosity.
* ICHECK	Convergence checking interval.
* ICTEST	Flag for convergence criteria to be used.
* IDTAU	Flag for time step selection method.
* IHSTAG	Flag for constant stagnation enthalpy option.
* ISWIRL	Flag for swirl in axisymmetric flow.
IT	Current time step number n .
ITBEG	The time level n at the beginning of a run.
* LR, UR	Reference length L_r and velocity u_r .
NEQ	Number of coupled equations being solved, N_{eq} .
* NHIST	Unit number for convergence history file.
* NITAVG	Number of time steps in moving average convergence test.
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
NTOTP	Dimensioning parameter specifying the storage required for a full two-dimensional array (i.e., $N1P \times N2P$).
NVD, NPTSD	Leading two dimensions for the array S.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
N1P, N2P	Parameters specifying the dimension sizes in the ξ and η directions.
S	Source term subvector S for first ADI sweep.
TAU	Current time value τ .

Output

LRMAX	Grid indices i and j , in the ξ and η directions, corresponding to the location of RESMAX.
RESAVG	The average absolute value of the residual, R_{avg} .
RESL2	The L_2 norm of the residual, R_{L_2} .
RESMAX	The maximum absolute value of the residual, R_{max} .

Description

Subroutine RESID computes various measures of the residual, and writes the convergence history file.

For problems without artificial viscosity, the steady-state form of the governing partial differential equations can be written as

$$0 = -\frac{\partial \hat{\mathbf{E}}}{\partial \xi} - \frac{\partial \hat{\mathbf{F}}}{\partial \eta} + \frac{\partial \hat{\mathbf{E}}_V}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}_V}{\partial \eta}$$

The residual is defined as the number resulting from evaluating the right hand side of the above equation. For first-order time differencing, this is simply the source term for the first ADI sweep, divided by the time step $\Delta\tau$.³² The residual at a specific grid point and time level is thus

$$R_{i,j}^n = S_{i,j}^n / (\Delta\tau)_{i,j}^n$$

where S is the source term for the first ADI sweep. Separate residuals are computed for each governing equation.

Adding artificial viscosity, however, changes the governing equations. With artificial viscosity, the difference equations actually correspond to the following differential equations at steady state.³³

$$\begin{aligned} 0 = & -\frac{\partial \hat{\mathbf{E}}}{\partial \xi} - \frac{\partial \hat{\mathbf{F}}}{\partial \eta} + \frac{\partial \hat{\mathbf{E}}_V}{\partial \xi} + \frac{\partial \hat{\mathbf{F}}_V}{\partial \eta} \\ & + \frac{\varepsilon_E^{(2)}}{J} \left[(\Delta\xi)^2 \frac{\partial^2 (J\hat{\mathbf{Q}})}{\partial \xi^2} + (\Delta\eta)^2 \frac{\partial^2 (J\hat{\mathbf{Q}})}{\partial \eta^2} \right] \\ & - \frac{\varepsilon_E^{(4)}}{J} \left[(\Delta\xi)^4 \frac{\partial^4 (J\hat{\mathbf{Q}})}{\partial \xi^4} + (\Delta\eta)^4 \frac{\partial^4 (J\hat{\mathbf{Q}})}{\partial \eta^4} \right] \end{aligned}$$

For cases run with artificial viscosity, therefore, the residual should include the explicit artificial viscosity terms. The implicit terms do not appear, since they difference $\Delta\hat{\mathbf{Q}}$, and in the steady form of the equations $\Delta\hat{\mathbf{Q}} = 0$. Since the explicit artificial viscosity terms are added to the source term for the first ADI sweep, they are automatically included in the residual.

Three measures of the residual are computed for each governing equation - the L_2 norm of the residual, the average absolute value of the residual, and the maximum absolute value of the residual. In addition, the (ξ, η) indices corresponding to the location of the maximum residual are saved. The L_2 norm of the residual is defined as

³² See equation (8.5a) in Volume 1. For first-order time differencing, $\theta_2 = \theta_3 = 0$.

³³ These equations represent the use of the constant coefficient artificial viscosity model. The nonlinear coefficient model is more complicated, but the same principle applies.

$$R_{L_2} = \left(\sum (R_{i,j})^2 \right)^{1/2}$$

In computing the residuals, the summations, maximums, and averages are over all interior grid points, plus points on spatially periodic boundaries.

For cases run with artificial viscosity, subroutine RESID is called from EXEC both before and after the artificial viscosity terms have been added to the equations. The residuals are thus computed both with and without the artificial viscosity terms. This may provide some estimate of the overall error in the solution introduced by the artificial viscosity. Convergence is determined by the residuals with the artificial viscosity terms included.

In addition to computing the residuals, subroutine RESID writes the convergence history file. The contents and format of this file are described in detail in Section 4.3 of Volume 2.

Remarks

1. The Cray BLAS routines SNRM2 and SASUM are used in computing the L_2 norm of the residual and the average absolute value of the residual, respectively. The Cray search routine ISAMAX is used in computing the maximum absolute value of the residual.
2. The scratch array DUMMY, from the common block DUMMY1, is used to store the values of the residual at each grid point.

Subroutine REST (IOPT)		
Called by	Calls	Purpose
INITC MAIN	METS	Read and/or write restart file.

Input When Reading the Restart File

* GAMR	Reference ratio of specific heats, γ_r .
* HSTAG	Stagnation enthalpy h_T used with constant stagnation enthalpy option.
* IHSTAG	Flag for constant stagnation enthalpy option.
IOPT	Flag specifying I/O operation; 1 to read, 2 to write.
* ITURB	Flag for turbulent flow option.
* NRQIN	Unit number for reading the restart flow field.
* NRXIN	Unit number for reading the restart computational mesh.
RGAS	Dimensionless gas constant R .

Input When Writing the Restart File

E, KE	Turbulent dissipation rate ε and kinetic energy k at time level $n + 1$.
EL, KEL	Turbulent dissipation rate ε and kinetic energy k at time level n .
IOPT	Flag specifying I/O operation; 1 to read, 2 to write.
IT	Current time step number n .
* ITURB	Flag for turbulent flow option.
* MACHR	Reference Mach number M_r .
* NRQOUT	Unit number for writing the restart flow field.
* NRXOUT	Unit number for writing the restart computational mesh.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
* RER	Reference Reynolds number Re_r .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level $n + 1$.
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
TAU	Computational time τ at time level $n + 1$.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output When Reading the Restart File

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
E, KE	Turbulent dissipation rate ε and kinetic energy k at time level ITBEG.

EL, KEL	Turbulent dissipation rate ε and kinetic energy k at time level ITBEG - 1.
ITBEG	The time level n at the beginning of the new run.
MACHR	Reference Mach number M_r .
N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
RER	Reference Reynolds number Re_r .
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level ITBEG.
RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at time level ITBEG - 1.
T, TL	Static temperature T at time levels ITBEG and ITBEG - 1.
TAU	Computational time τ at time level ITBEG.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output When Writing the Restart File

None.

Description

Subroutine REST reads and/or writes the restart files. Restarting a calculation requires two unformatted files - one containing the computational mesh and one containing the flow field.

If subroutine REST is being used to read the restart files, the computational mesh is first read from unit NRXIN. The grid increments $\Delta\xi$ and $\Delta\eta$ are then set, and subroutine METS is called to compute the metric coefficients and the Jacobian of the grid transformation.

The flow field file is read next, from unit NRQIN. It normally contains the results at the last two time levels that were computed during the previous run. If only one level is present in the file, however, the results at level $n - 1$ are set equal to those at level n . If the previous run used the two-equation turbulence model, the turbulence variables are also read from the file. The beginning time level for the time marching loop is set equal to the level stored in the restart file. The flow field variables in the restart file are the conservation variables Q , nondimensionalized as in the plotting program PLOT3D.³⁴ They therefore must be converted into the primitive variables used in *Proteus*. The temperature is then computed from the perfect gas equation of state, with c_p and c_v defined using the input reference conditions.

When writing the restart files, the file containing the computational mesh is written onto unit NRXOUT. The primitive flow variables are then redefined as conservation variables and nondimensionalized as in PLOT3D. They are then written onto unit NRQOUT. If the current run used the two-equation turbulence model, the turbulence variables are also written into the file.

Remarks

1. If, in the input namelist RSTRT, NRXOUT and NRQOUT are set equal to NRXIN and NRQIN, respectively, the output restart files will overwrite the input restart files.
2. Except for the turbulence variables and the variables at time level $n - 1$, the restart files have the same format as the XYZ and Q files created using the IPLOT = 2 and 3 options. These restart files can thus also be used as XYZ and Q files for the PLOT3D plotting program. Since $N3 = 1$, the $n - 1$ level will not be read by PLOT3D.

³⁴ See Sections 4.2.3 and 4.4 of Volume 2.

3. The temperature T is computed using the equation of state, which contains a specific heat coefficient (either c_p or c_v , depending on whether the stagnation enthalpy is assumed constant or not.) In subroutine REST, a constant value of specific heat is used, consistent with the reference temperature T_r . If the user specified constant specific heat (i.e., a value for γ , was read in), this is not a problem. However, if the temperature-dependent specific heat option is being used (i.e., a value for γ , was not read in), the equation of state and the empirical equation for specific heat are coupled. For this reason, in INITC (the routine that calls REST), T is recomputed by calling EQSTAT after the specific heats have been computed in FTEMP. Ideally, this coupling would be handled by iteration between FTEMP and EQSTAT. This is not currently done in *Proteus*, however.

Subroutine ROBTS (NP,A,B,XP)		
Called by	Calls	Purpose
PAK		Pack points along a line using Roberts transformation.

Input

A	Parameter α in Roberts transformation formula specifying location of packing: 0.0 to pack near $x_P = 1$ only, 1.0 to pack near $x_P = 0$ only, and 0.5 to pack equally at $x_P = 0$ and 1.0.
B	Parameter β in Roberts transformation formula specifying amount of packing. A value approaching 1.0 from above gives denser packing.
NP	Number of grid points along the line.

Output

XP	Coordinates of packed grid points along the line.
----	---

Description

Subroutine ROBTS packs points along a line of length one using a transformation due to Roberts (1971). The basic transformation is given by

$$x_P = \frac{(\beta + 2\alpha)\beta_r^{\beta_x} - \beta + 2\alpha}{(2\alpha + 1)(1 + \beta_r^{\beta_x})}$$

where

$$\beta_r = \frac{\beta + 1}{\beta - 1}$$

$$\beta_x = \frac{x_{UP} - \alpha}{1 - \alpha}$$

and x_P and x_{UP} are the packed and unpacked (i.e., evenly spaced) coordinates along the line. The parameter α determines the packing location. For $\alpha = 0$, the points will be packed only near $x_P = 1$, and for $\alpha = 1/2$ the points will be packed equally near $x_P = 0$ and $x_P = 1$. The packing parameter β determines the amount of packing. It is a number greater than 1, but generally 1.1 or below. The closer β is to 1, the tighter the packing will be.

It may seem logical to set $\alpha = 1$ to pack points near $x_P = 0$. With the basic transformation, however, this doesn't work. In *Proteus* we get around this problem by replacing α in the above transformation with α_w , where $\alpha_w = \alpha$ if $\alpha = 0$ or $1/2$, and $\alpha_w = 0$ if $\alpha = 1$. If $\alpha = 0$ or $1/2$, no further action is necessary. If $\alpha = 1$, however, we must invert the resulting x_P values and re-order the indices. I.e., for $i = 1$ to NP, we set

$$(x_{PI})_i = 1 - (x_P)_i$$

After this operation, the array x_{PI} will run from 1 to 0, packed near 1. To re-order the indices, for $i = 1$ to NP we set

$$(x_P)_{NP-i+1} = (x_{PI})_i$$

After this operation, x_P will run from 0 to 1, packed near 0.

Finally, to ensure round-off error doesn't affect the endpoint values, we set $(x_P)_1 = 0$ and $(x_P)_{NP} = 1$.

Remarks

1. The namelist input variable $SQ(IDIR,1)$, which is used to specify the packing location in direction $IDIR$, is actually equal to $1 - \alpha$. Therefore, setting $SQ(IDIR,1) = 0$ results in packing near the ξ or $\eta = 0$ boundary, and $SQ(IDIR,1) = 1$ results in packing near the ξ or $\eta = 1$ boundary.

Function SASUM (N,V,INC)		
Called by	Calls	Purpose
RESID		Compute the sum of the absolute values of the elements of a vector.

Input

N	Number of elements in the vector to be summed.
V	Vector to be summed.
INC	Skip distance between elements of V. For contiguous elements, INC = 1.

Output

SASUM	Sum of the absolute values of the elements of V.
-------	--

Description

Function SASUM computes the sum of the absolute values of the elements of a vector. For a one-dimensional vector, the use of SASUM is straightforward. For example,

$$\text{sasum}(\text{np}, \text{v}, 1) = \sum_{i=1}^{\text{np}} V_i$$

A starting location can be specified, as in

$$\text{sasum}(\text{np}-4, \text{v}(5), 1) = \sum_{i=5}^{\text{np}} V_i$$

Multi-dimensional arrays can be used by taking advantage of the way Fortran arrays are stored in memory, and specifying the proper vector length and skip distance. For instance, if A is an array dimensioned NDIM1 by NDIM2, then

$$\text{sasum}(\text{ndim1} \times \text{ndim2}, \text{a}, 1) = \sum_{i=1}^{\text{ndim1}} \sum_{j=1}^{\text{ndim2}} A_{i,j}$$

One dimension at a time can also be summed. For example,

$$\text{sasum}(\text{ndim1}, \text{a}(1,5), 1) = \sum_{i=1}^{\text{ndim1}} A_{i,5}$$

Similarly, by specifying a skip increment,

$$\text{sasum}(\text{ndim2}, \text{a}(5,1), \text{ndim1}) = \sum_{j=1}^{\text{ndim2}} A_{5,j}$$

Remarks

1. SASUM is a Cray BLAS (Basic Linear Algebra Subprograms) routine (Cray Research, Inc., 1989b).

Subroutine SGEFA (A,LDA,N,IPVT,INFO)		
Called by	Calls	Purpose
BCELIM BVUP	ISAMAX	Factor a matrix using Gaussian elimination.

Input

A	An array containing the matrix A to be factored, dimensioned as A(LDA,N).
LDA	The leading dimension of the array A.
N	The order of the matrix A.

Output

A	An upper triangular matrix and the multipliers which were used to obtain it. The factorization can be written as $A = LU$, where L is a product of permutation and unit lower triangular matrices, and U is upper triangular.
IPVT	A vector of length N containing pivot indices.
INFO	An error flag: 0 for normal operation, k if $U_{kk} = 0$.

Description

Subroutine SGEFA is used in combination with subroutine SGESL to solve the matrix equation $Ax = B$. If the Fortran arrays A and B represent A and B, where A is a square N by N matrix and B is a matrix (or vector) with NCOL columns, and if the leading dimension of the Fortran array A is LDA, then the Fortran sequence

```

      call sgefa (a,lda,n,ipvt,info)
      do 10 j = 1,ncol
      call sgesl (a,lda,n,ipvt,b(1,j),0)
10    continue

```

computes $A^{-1}B$, storing the result in B.

Remarks

1. SGEFA is a Cray LINPACK routine (Cray Research, Inc., 1989b; Dongarra, Moler, Bunch, and Stewart, 1979).

Subroutine SGESL (A,LDA,N,IPVT,B,JOB)		
Called by	Calls	Purpose
BCELM BVUP		Solve the matrix equation $Ax = B$ or $A^T x = B$ using the factors computed by SGEFA.

Input

A	The two-dimensional output array A from SGEFA containing the factorization of matrix A.
B	The right-hand side vector B.
IPVT	The output array IPVT of pivot indices from SGEFA.
JOB	Flag specifying type of matrix equation: 0 to solve $Ax = B$; non-zero to solve $A^T x = B$.
LDA	The leading dimension of the array A.
N	The order of the matrix A.

Output

B	The solution vector x.
---	------------------------

Description

Subroutine SGESL is used in combination with subroutine SGEFA to solve the matrix equation $Ax = B$. See the description of subroutine SGEFA for details.

Remarks

1. SGESL is a Cray LINPACK routine (Cray Research, Inc., 1989b; Dongarra, Moler, Bunch, and Stewart, 1979).

Function SNRM2 (N,V,INC)		
Called by	Calls	Purpose
RESID		Compute the L_2 norm of a vector.

Input

N	The number of elements in the vector V.
V	The vector whose norm is to be computed.
INC	Skip distance between elements of V. For contiguous elements, INC = 1.

Output

SNRM2	The L_2 norm of the vector V.
-------	---------------------------------

Description

Function SNRM2 computes the L_2 norm of a vector. For a one-dimensional vector, the use of SNRM2 is straightforward. For example,

$$\text{snrm2}(\text{np}, \text{v}, 1) = \left(\sum_{i=1}^{\text{np}} V_i^2 \right)^{1/2}$$

A starting location can be specified, as in

$$\text{snrm2}(\text{np}-4, \text{v}(5), 1) = \left(\sum_{i=5}^{\text{np}} V_i^2 \right)^{1/2}$$

Multi-dimensional arrays can be used by taking advantage of the way Fortran arrays are stored in memory, and specifying the proper vector length and skip distance. For instance, if A is an array dimensioned NDIM1 by NDIM2, then

$$\text{snrm2}(\text{ndim1} \times \text{ndim2}, \text{a}, 1) = \left(\sum_{i=1}^{\text{ndim1}} \sum_{j=1}^{\text{ndim2}} A_{i,j}^2 \right)^{1/2}$$

One dimension at a time can also be summed. For example,

$$\text{snrm2}(\text{ndim1}, \text{a}(1, 5), 1) = \left(\sum_{i=1}^{\text{ndim1}} A_{i,5}^2 \right)^{1/2}$$

Similarly, by specifying a skip increment,

$$\text{snrm2}(\text{ndim2}, \mathbf{a}(5,1), \text{ndim1}) = \left(\sum_{j=1}^{\text{ndim2}} A_{5,j}^2 \right)^{1/2}$$

Remarks

1. SNRM2 is a Cray BLAS (Basic Linear Algebra Subprograms) routine (Cray Research, Inc., 1989b).

Subroutine TBC		
Called by	Calls	Purpose
MAIN		Set time-dependent boundary condition values.

Input

- * GTBC1, GTBC2 Time-dependent surface mean flow boundary condition values for the ξ and η directions.
- IT Current time step number n .
- ITBEG The time level n at the beginning of a run.
- ITEND Final time step number.
- * JBC1, JBC2 Surface mean flow boundary condition types for the ξ and η directions.
- * JTBC1, JTBC2 Flags for type of time dependency for mean flow boundary conditions in the ξ and η directions.
- NBC Dimensioning parameter specifying number of boundary conditions per equation.
- NEQ Number of coupled equations being solved, N_{eq} .
- * NOUT Unit number for standard output.
- * NTBC Number of values in tables for general unsteady boundary conditions.
- * NTBCA Time levels at which general unsteady boundary conditions are specified.
- * N1, N2 Number of grid points N_1 and N_2 , in the ξ and η directions.

Output

- FBC1, FBC2 Point-by-point mean flow boundary condition values for the ξ and η directions.
- GBC1, GBC2 Surface mean flow boundary condition values for the ξ and η directions.

Description

Subroutine TBC sets time-dependent mean flow boundary condition values. Two types of time dependency are allowed - general and periodic.

General Time-Dependent Boundary Conditions

General time-dependent boundary conditions are set using linear interpolation on an input table of boundary condition values vs. time level. Thus, the boundary condition value is

$$g^{n+1} = g_t^i + \frac{n+1-n_t^i}{n_t^{i+1}-n_t^i} (g_t^{i+1} - g_t^i)$$

Here n is the current known time level in the time marching scheme, g_i and n_i represent the input table of boundary condition values vs. time level, and i is the index in the table for which

$$n_t^i \leq n + 1 < n_t^{i+1}$$

If $n + 1 < n_t^1$, then g^{n+1} is set equal to the first value in the table, g_t^1 . Similarly, if $n + 1 > n_t^N$, where N is the index of the last entry in the table, then g^{n+1} is set equal to the last value in the table, g_t^N .

In Fortran, $g = \text{GBC1}$ or GBC2 , $g_t = \text{GTBC1}$ or GTBC2 , $n_t = \text{NTBCA}$, and $N = \text{NTBC}$.

Time-Periodic Boundary Conditions

Time-periodic boundary conditions (not to be confused with spatially periodic boundary conditions) are of the form

$$g^{n+1} = g_t^1 + g_t^2 \sin[g_t^3(n+1) + g_t^4]$$

where g_t^1 through g_t^4 are given by the first four elements of GTBC1 or GTBC2 .

Remarks

1. An error message is generated and execution is stopped if an invalid type of unsteadiness is requested for the boundary values.

Subroutine TIMSTP		
Called by	Calls	Purpose
MAIN	ISAMAX	Set computational time step.

Input

* CFL	CFL number in IDTAU = 1, 2, 5, 6, 8, and 9 options.
* CFLMIN, CFLMAX	Minimum and maximum CFL numbers allowed in IDTAU = 2 and 6 options.
CHGMAX	Maximum change in absolute value of the dependent variables over previous time step (or NITAVG - 1 time steps if ICTEST = 2), ΔQ_{max} .
* CHG1, CHG2	Minimum and maximum change, in absolute value, that is allowed in any dependent variable before increasing or decreasing $\Delta\tau$ in IDTAU = 2, 4, and 6 options.
CP, CV	Specific heats c_p and c_v at time level n .
* DT	Time step $\Delta\tau$ in IDTAU = 3 and 4 options.
DTAU	Old computational time step $\Delta\tau$.
* DTF1, DTF2	Factors multiplying or dividing $\Delta\tau$ if solution changes too slowly or quickly in IDTAU = 2, 4, and 6 options.
* DTMIN, DTMAX	Minimum and maximum $\Delta\tau$ allowed in IDTAU = 4 option, or used in IDTAU = 7 option.
DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY, ETAT	Metric coefficients η_x , η_y (or η_r if axisymmetric), and η_t .
* IDTAU	Flag for time step selection method.
IT	Current time step number n .
ITSEQ	Current time step sequence number.
MU	Effective coefficient of viscosity μ at time level n .
* NDTCYC	Number of time steps per cycle for IDTAU = 7 option.
NEQ	Number of coupled equations being solved, N_{eq} .
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
* RER	Reference Reynolds number Re_r .
RGAS	Gas constant R .
RHO, U, V	Static density ρ , and velocities u and v , at time level n .
T	Static temperature T at time level n .
XIX, XIY, XIT	Metric coefficients ξ_x , ξ_y (or ξ_r if axisymmetric), and ξ_t .

Output

CFL	New CFL number in IDTAU = 2 and 6 options.
DTAU	New computational time step $\Delta\tau$.

Description

Subroutine TIMSTP computes the time step size $\Delta\tau$. The following sections describe the various methods currently available for setting and/or modifying $\Delta\tau$.

IDTAU = 1

This option sets a global (i.e., constant in space) time step $\Delta\tau$ equal to the minimum of the values at each grid point computed from the input parameter CFL(ITSEQ). I.e.,

$$\Delta\tau = (\text{CFL}) \min_{i,j} (\Delta\tau_{cfl})$$

where $\Delta\tau_{cfl}$ is the inviscid CFL limit, given in generalized two-dimensional coordinates as (Shang, 1984).

$$\Delta\tau_{cfl} = \left\{ \left| \frac{U}{\Delta\xi} \right| + \left| \frac{V}{\Delta\eta} \right| + a \left[\left(\frac{\xi_x}{\Delta\xi} + \frac{\eta_x}{\Delta\eta} \right)^2 + \left(\frac{\xi_y}{\Delta\xi} + \frac{\eta_y}{\Delta\eta} \right)^2 \right]^{1/2} \right\}^{-1}$$

Here $U = \xi_t + \xi_x u + \xi_y v$ and $V = \eta_t + \eta_x u + \eta_y v$ are the contravariant velocities without metric normalization, and $a = \sqrt{\gamma RT}$ is the speed of sound.

IDTAU = 2

For the first time step, this option is identical to the IDTAU = 1 option. After the first time step, however, CFL is modified to keep ΔQ_{max} , the maximum change in absolute value of the dependent variables, within user-specified limits. The rules used to increase or decrease CFL may be summarized as follows:

$$\begin{aligned} \Delta Q_{max} < \text{CHG1} &\Rightarrow \text{CFL} = \min[(\text{DTF1})(\text{CFL}), \text{CFLMAX}] \\ \Delta Q_{max} > \text{CHG2} &\Rightarrow \text{CFL} = \max[\text{CFL}/\text{DTF2}, \text{CFLMIN}] \\ \Delta Q_{max} > 0.15 &\Rightarrow \text{CFL} = \text{CFL}/2 \end{aligned}$$

The time step $\Delta\tau$ is then set using the same formulas as in the IDTAU = 1 option.

IDTAU = 3

This option sets a global (i.e., constant in space) time step $\Delta\tau$ equal to the input parameter DT(ITSEQ).

IDTAU = 4

For the first time step, this option is identical to the IDTAU = 3 option. After the first time step, however, $\Delta\tau$ is modified to keep ΔQ_{max} , the maximum change in absolute value of the dependent variables, within user-specified limits. The rules used to increase or decrease $\Delta\tau$ may be summarized as follows:

$$\begin{aligned} \Delta Q_{max} < \text{CHG1} &\Rightarrow \Delta\tau = \min[(\text{DTF1})\Delta\tau, \text{DTMAX}] \\ \Delta Q_{max} > \text{CHG2} &\Rightarrow \Delta\tau = \max[\Delta\tau/(\text{DTF2}), \text{DTMIN}] \\ \Delta Q_{max} > 0.15 &\Rightarrow \Delta\tau = \Delta\tau/2 \end{aligned}$$

IDTAU = 5

This option sets a local (i.e., varying in space) time step $\Delta\tau$ computed at each grid point from the input parameter CFL(ITSEQ). I.e., at each grid point,

$$\Delta\tau = (\text{CFL})\Delta\tau_{cfl}$$

where $\Delta\tau_{cfl}$ is given above in the description of the IDTAU = 1 option.

IDTAU = 6

For the first time step, this option is identical to the IDTAU = 5 option. After the first time step, however, CFL is modified to keep ΔQ_{max} , the maximum change in absolute value of the dependent variables, within user-specified limits. The rules used to increase or decrease CFL are the same as in the IDTAU = 2 option.

IDTAU = 7

This option sets a global (i.e., constant in space) time step $\Delta\tau$ with logarithmic cycling. The formula used is

$$\Delta\tau = \Delta\tau_{min} \left(\frac{\Delta\tau_{max}}{\Delta\tau_{min}} \right)^{N/(N_{cyc} - 1)}$$

where $N = \text{mod}(n - 1, N_{cyc})$ and n is the current known time level. The time step $\Delta\tau$ is thus cycled repeatedly between $\Delta\tau_{min}$ and $\Delta\tau_{max}$ every N_{cyc} time steps. The values of $\Delta\tau_{min}$, $\Delta\tau_{max}$, and N_{cyc} are given by the input parameters DTMIN, DTMAX, and NDTCCY.

IDTAU = 8

This option sets a local (i.e., varying in space) time step $\Delta\tau$ computed at each grid point using the procedure of Knight and Choi (1989). The inviscid CFL limit $\Delta\tau_{cfl}$ is first computed separately for each computational coordinate direction. Thus, at each grid point,

$$(\Delta\tau_{cfl})_{\xi} = \left[\left| \frac{U}{\Delta\xi} \right| + a \frac{\sqrt{\xi_x^2 + \xi_y^2}}{\Delta\xi} \right]^{-1}$$
$$(\Delta\tau_{cfl})_{\eta} = \left[\left| \frac{V}{\Delta\eta} \right| + a \frac{\sqrt{\eta_x^2 + \eta_y^2}}{\Delta\eta} \right]^{-1}$$

Here $U = \xi_t + \xi_x u + \xi_y v$ and $V = \eta_t + \eta_x u + \eta_y v$ are the contravariant velocities without metric normalization, and $a = \sqrt{\gamma RT}$ is the speed of sound.

A preliminary value of $\Delta\tau$ is then defined at each grid point using the input parameter CFL(ITSEQ).

$$\Delta\tau_0 = (\text{CFL}) \min[(\Delta\tau_{cfl})_{\xi}, (\Delta\tau_{cfl})_{\eta}]$$

The final value of $\Delta\tau$ is then defined at each grid point as

$$\Delta\tau = \max[\Delta\tau_0, (\Delta\tau_{cfl})_{\xi}]$$

Knight and Choi found that using this definition for $\Delta\tau$, rather than simply setting $\Delta\tau = \Delta\tau_0$, resulted in faster convergence for problems with refined grid regions. This formulation assumes that flow is generally in the ξ direction.

IDTAU = 9

This option is similar to the IDTAU = 8 option. The only difference is a viscous correction added to the definitions of the inviscid CFL limits, similar to that used by Cooper (1987). The inviscid CFL limits are now defined at each grid point as:

$$(\Delta\tau_{cfl})_{\xi} = \left[\left| \frac{U}{\Delta\xi} \right| + a \frac{\sqrt{\xi_x^2 + \xi_y^2}}{\Delta\xi} + \frac{2}{Re_r} \frac{\mu}{\rho} \frac{\xi_x^2 + \xi_y^2}{(\Delta\xi)^2} \right]^{-1}$$

$$(\Delta\tau_{cfl})_{\eta} = \left[\left| \frac{V}{\Delta\eta} \right| + a \frac{\sqrt{\eta_x^2 + \eta_y^2}}{\Delta\eta} + \frac{2}{Re_r} \frac{\mu}{\rho} \frac{\eta_x^2 + \eta_y^2}{(\Delta\eta)^2} \right]^{-1}$$

The rest of the procedure for computing $\Delta\tau$ is the same as in the IDTAU = 8 option.

Remarks

1. In ΔQ_{max} , used in the IDTAU = 2, 4, and 6 options, the change in E_T has been divided by $R/(\gamma_r - 1) + 1/2$. This is equivalent to dividing the dimensional value \bar{E}_T by

$$E_{T_r} = \frac{\rho_r \bar{R} T_r}{\gamma_r - 1} + \frac{\rho_r u_r^2}{2}$$

This makes the change in total energy the same order of magnitude as the other conservation variables.

2. An error message is generated and execution is stopped if an illegal time step selection option is requested.
3. A warning message is printed with the IDTAU = 2, 4, and 6 options if $\Delta\tau$ or the CFL number is cut in half because $\Delta Q_{max} > 0.15$.
4. The Cray search routine ISAMAX is used in computing the maximum value of ΔQ_{max} for all the equations.

Subroutine TREMAIN (CPUREM)		
Called by	Calls	Purpose
MAIN		Get CPU time remaining for the job.

Input

None.

Output

CPUREM Amount of CPU time remaining, in seconds.

Description

Subroutine TREMAIN computes the amount of CPU time remaining for the current job, in seconds.

Remarks

1. TREMAIN is a Cray Fortran library routine (Cray Research, Inc., 1989a).

Subroutine TURBBL		
Called by	Calls	Purpose
INITC KEINIT MAIN	BLIN1 BLIN2 BLOUT1 BLOUT2 VORTEX	Manage computation of turbulence parameters using Baldwin-Lomax algebraic model.

Input

CP	Specific heat c_p .
* ITETA, ITXI	Flags for computation of turbulent viscosity along constant η and ξ lines.
* KBC1, KBC2	Boundary types for the ξ and η directions.
* LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries.
LWSET	Flags specifying how wall locations are to be determined for the turbulence model; 0 if wall locations are to be found automatically by searching for boundary points where the velocity is zero, 1 if input using the LWALL parameters, 2 if input using the IWALL parameters.
MU, LA, KT	Laminar coefficient of viscosity μ_l , laminar second coefficient of viscosity λ_l , and laminar coefficient of thermal conductivity k_l .
* NOUT	Unit number for standard output.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
PRR	Reference Prandtl number Pr_r .
* PRT	Turbulent Prandtl number Pr_t , or, if $PRT \leq 0$, a flag indicating the use of a variable turbulent Prandtl number.
* RER	Reference Reynolds number Re_r .
* REXT1, REXT2	Transition Reynolds numbers Re_{x_t} in the ξ and η directions.
RHO, U, V, W	Static density ρ , and velocities u , v , and w .
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries, if not set in input.
MU, LA, KT	Effective coefficient of viscosity μ , effective second coefficient of viscosity λ , and effective coefficient of thermal conductivity k .
MUT	Turbulent viscosity coefficient μ_t .

Description

Subroutine TURBBL manages the computation of the effective coefficient of viscosity, second coefficient of viscosity, and coefficient of thermal conductivity using the algebraic eddy viscosity model of Baldwin and Lomax (1978). It is called from MAIN during each step from time level n to $n + 1$, but after the governing flow equations have been solved. The Fortran variables RHO, U, etc., are thus at the $n + 1$

level. The effective viscosity coefficient to be computed will therefore also be at the $n + 1$ level. This, of course, becomes the known n level for the next time step.

The steps involved in computing the effective coefficients are as follows:

1. Initialize the arrays for storing the turbulent viscosity μ_t on constant ξ and η lines to zero.
2. Call VORTEX to compute $|\bar{\Omega}|$, the magnitude of the total vorticity vector.
3. At each ξ location, compute μ_t due to walls at $\eta = 0$ and/or $\eta = 1$, or due to a free turbulent flow in the ξ direction, using steps 3a - 3c. The result will be stored in the Fortran array MUT. If bypassing the calculation on constant ξ lines, skip to step 4 to compute μ_t on constant η lines.
 - 3a. Determine wall locations by checking for zero velocity at the η boundaries, unless wall locations are user-specified via the input LWALL or IWALL parameters, or unless boundary types are specified using the KBC parameters.
 - 3b. Call BLOUT1 to compute $(\mu_t)_{outer}$, at the current ξ location, for $\eta = 0$ to 1.
 - 3c. Call BLIN1 to compute $(\mu_t)_{inner}$, at the current ξ location, within the inner region for a solid wall at $\eta = 0$ and/or $\eta = 1$.
4. At each η location, compute μ_t due to walls at $\xi = 0$ and/or $\xi = 1$, or due to a free turbulent flow in the η direction, using steps 4a - 4c. The result will be stored in the Fortran array DUMMY. If bypassing the calculation on constant η lines, skip to step 5.
 - 4a. Determine wall locations by checking for zero velocity at the ξ boundaries, unless wall locations are user-specified via the input LWALL or IWALL parameters, or unless boundary types are specified using the KBC parameters.
 - 4b. Call BLOUT2 to compute $(\mu_t)_{outer}$, at the current η location, for $\xi = 0$ to 1.
 - 4c. Call BLIN2 to compute $(\mu_t)_{inner}$, at the current η location, within the inner region for a solid wall at $\xi = 0$ and/or $\xi = 1$.
5. If the input is such that the computation of μ_t is bypassed in both directions, write an error message and stop.
6. If μ_t is being computed on constant ξ lines only, then $MUT = \mu_t$, so skip to step 9.
7. If μ_t is being computed on constant η lines only, then $DUMMY = \mu_t$, so set $MUT = DUMMY$ and skip to step 9.
8. If μ_t is being computed both on constant ξ lines and constant η lines, compute a single μ_t value at each grid point using the averaging formula presented in equation (9.13) of Volume 1.
9. If specified in the input, modify μ_t to account for laminar-turbulent transition using a model based on one given by Cebeci and Bradshaw (1984). This model is described in Section 9.1.4 of Volume 1.
10. Define the necessary effective coefficients as follows:

$$\begin{aligned}\mu &= \mu_l + \mu_t \\ \lambda &= \lambda_l + \lambda_t \\ k &= k_l + k_t\end{aligned}$$

where $\lambda_t = -2\mu_t/3$, and k_t is computed using Reynold's analogy as

$$k_t = \frac{\mu_t c_p}{Pr_t} Pr_r$$

The turbulent Prandtl number is either a constant specified in the input, or a variable computed using equation (9.19) of Volume 1.

Remarks

1. In the averaging formula used when μ_t is computed both on constant ξ lines and constant η lines, the Fortran variables F1 and F2 are

$$F1 = \frac{(y_n)_2}{[(y_n)_1^2 + (y_n)_2^2]^{1/2}}$$

$$F2 = \frac{(y_n)_1}{[(y_n)_1^2 + (y_n)_2^2]^{1/2}}$$

If $(y_n)_1$ and $(y_n)_2$ are both close to zero, F1 and F2 are set equal to $1/\sqrt{2}$, which is the limiting value in the above equations as $(y_n)_1$ and $(y_n)_2$ approach zero.

2. The exponent in the definition of γ_{tr} is limited to 20.
3. In the Fortran equation for the effective thermal conductivity, the factor $PRR = Pr$, is necessary for proper nondimensionalization of k_t .
4. The distance used in the formula for γ_{tr} is a straight-line distance from one point to another. It would probably be better to compute a curvilinear distance along the coordinate line.
5. The scratch array DUMMY, from the common block DUMMY1, is used to store the value of the turbulent viscosity along constant η lines. The array is filled in subroutines BLIN2 and BLOUT2.
6. If ITXI and ITETA are both zero, indicating the turbulent viscosity computation is to be bypassed for both coordinate directions, an error message is generated and execution is stopped.

Subroutine TURBCH		
Called by	Calls	Purpose
MAIN	EXECT PRODC YPLUSN	Manage computation of turbulence parameters using the Chien k - ϵ model.

Input

CP	Specific heat c_p .
* KBC1, KBC2	Boundary types for the ξ and η directions.
* LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries.
LWSET	Flags specifying how wall locations are to be determined for the turbulence model; 0 if wall locations are to be found automatically by searching for boundary points where the velocity is zero, 1 if input using the LWALL parameters, 2 if input using the IWALL parameters.
MU, LA, KT	Laminar coefficient of viscosity μ_l , laminar second coefficient of viscosity λ_l , and laminar coefficient of thermal conductivity k_l .
MUT	Turbulent viscosity μ_t at time level n .
* NTKE	Number of k - ϵ iterations per mean flow iteration.
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
PRR	Reference Prandtl number Pr_r .
* PRT	Turbulent Prandtl number Pr_t , or, if $PRT \leq 0$, a flag indicating the use of a variable turbulent Prandtl number.
U, V, W	Velocities u , v , and w at time level n .

Output

LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries, if not set in input.
MU, LA, KT	Effective coefficient of viscosity μ , effective second coefficient of viscosity λ , and effective coefficient of thermal conductivity k .
MUT	Turbulent viscosity μ_t at time level n .

Description

Subroutine TURBCH manages the computation of the effective coefficient of viscosity, second coefficient of viscosity, and coefficient of thermal conductivity using the low Reynolds number k - ϵ two-equation turbulence model of Chien (1982). The k - ϵ equations are uncoupled from the mean flow equations, lagged in time and solved separately. This allows maximum modularity in turbulence modeling.

For each step from time level n to $n + 1$, the mean flow equations are solved first, using a time step $\Delta\tau$. The k - ϵ equations are then solved, using NTKE time steps with a time step size of TFACT($\Delta\tau$).

The steps involved in computing the effective coefficients are as follows:

1. Determine wall locations by checking for zero velocity at the boundaries, unless wall locations are user-specified via the input LWALL or IWALL parameters, or unless boundary types are specified using the KBC parameters.
2. Call YPLUSN to compute the minimum distance to the nearest solid wall and y^+ . To save storage, the minimum distance is returned in the Fortran variable DUMMY.
3. Call PRODCCT to compute the production rate of turbulent kinetic energy. To save storage space, the production rate is returned in the Fortran variable VORT.
4. Call EXECT to advance the k - ε equations in time using a time step of TFACT($\Delta\tau$).
5. Repeat steps 3-4 NTKE times.
6. Define the necessary effective coefficients as follows:

$$\begin{aligned}\mu &= \mu_l + \mu_t \\ \lambda &= \lambda_l + \lambda_t \\ k &= k_l + k_t\end{aligned}$$

where $\lambda_t = -2\mu_t/3$, and k_t is computed using Reynold's analogy as

$$k_t = \frac{\mu_t c_p}{Pr_t} Pr_t$$

The turbulent Prandtl number is either a constant specified in the input, or a variable computed using equation (9.19) of Volume 1.

Remarks

1. The scratch array DUMMY, from the common block DUMMY1, is used to store the values of the minimum distance to the nearest wall. The array is filled in subroutine YPLUSN.
2. The Fortran array VORT, from the common block TURB1, is used to store the values of the production rate of turbulent kinetic energy. The array is filled in subroutine PRODCCT.
3. For equal mean flow and k - ε time steps, use TFACT = 1/NTKE.

Subroutine UPDATE (S,NVD,NPTSD)		
Called by	Calls	Purpose
EXEC		Update flow variables after each ADI sweep.

Input

IBASE, ISTEP	Base index and multiplication factor used in computing one-dimensional index for two-dimensional array.
* IHSTAG	Flag for constant stagnation enthalpy option.
* ISWIRL	Flag for swirl in axisymmetric flow.
IV	Index in the "vectorized" direction, i .
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
NPTS	Number of grid points in the sweep direction, N .
NR, NRU, NRV, NRW, NET	Array indices associated with the dependent variables ρ , ρu , ρv , ρw , and E_T .
NVD, NPTSD	Leading two dimensions for the array S.
RHO, U, V, W, ET	Static density ρ , velocities u , v , and w , and total energy E_T at time level n .
S	Computed solution subvector, $\Delta\hat{Q}$.

Output

RHOL, UL, VL, WL, ETL	Static density ρ , velocities u , v , and w , and total energy E_T at end of current ADI sweep.
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Description

Subroutine UPDATE computes the primitive flow variables from the dependent variables $\Delta\hat{Q}$ after each ADI sweep. For the first sweep the formulas are

$$\begin{aligned}\rho^* &= \rho^n + J\Delta\hat{Q}_1^* \\ u^* &= \frac{1}{\rho^*} (\rho^n u^n + J\Delta\hat{Q}_2^*) \\ v^* &= \frac{1}{\rho^*} (\rho^n v^n + J\Delta\hat{Q}_3^*) \\ w^* &= \frac{1}{\rho^*} (\rho^n w^n + J\Delta\hat{Q}_4^*) \\ E_T^* &= E_T^n + J\Delta\hat{Q}_5^*\end{aligned}$$

where $\Delta\hat{Q}_1$ through $\Delta\hat{Q}_5$ are the dependent variables in delta form for the five governing equations.³⁵ For the second ADI sweep, the superscript * should be changed to $n + 1$ on ρ , u , v , w , and E_T , and to n on $\Delta\hat{Q}$.

Remarks

1. This subroutine uses one-dimensional addressing of two-dimensional arrays, as described in Section 2.3.

³⁵ These formulas are written for the most general case - axisymmetric flow with swirl and non-constant stagnation enthalpy. For simpler cases there may be only three or four equations.

Subroutine UPDTKE		
Called by	Calls	Purpose
EXECT		Update k and ε after each ADI sweep.

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
E	Turbulent dissipation rate ε at time level n .
FBCT1, FBCT2	Point-by-point k - ε boundary condition values for the ξ and η directions.
IBCT1, IBCT2	Point-by-point k - ε boundary condition types for the ξ and η directions.
JI	Inverse Jacobian of the nonorthogonal grid transformation, J^{-1} .
KBCPER	Flags for spatially periodic boundary conditions in the ξ and η directions.
KE	Turbulent kinetic energy k at time level n .
NPT1, NPT2	N_1 and N_2 for non-periodic boundary conditions, $N_1 + 1$ and $N_2 + 1$ for spatially periodic boundary conditions in ξ and η .
RHO	Static density ρ at time level n .
S	Computed solution subvector $\Delta\hat{W}$.

Output

E, EL	Turbulent dissipation rate ε at time levels $n + 1$ and n .
KE, KEL	Turbulent kinetic energy k at time levels $n + 1$ and n .

Description

Subroutine UPDTKE computes the primitive flow variables k and ε from the dependent variables $\Delta\hat{W}^n$ after a complete time step. The formulas are

$$k^{n+1} = \frac{1}{\rho^{n+1}} (\rho^{n+1} k^n + J \Delta\hat{W}_1^n)$$

$$\varepsilon^{n+1} = \frac{1}{\rho^{n+1}} (\rho^{n+1} \varepsilon^n + J \Delta\hat{W}_2^n)$$

where $\Delta\hat{W}_1$ and $\Delta\hat{W}_2$ are the dependent variables in delta form for the k - ε equations.

Subroutine UPDTKE also explicitly computes the k and ε values on the computational boundaries using the specified boundary conditions, as described below.

No Change From Initial Conditions, $\Delta k = 0$ and/or $\Delta \varepsilon = 0$

Values for k and ε are simply not updated. Therefore, their values on the boundaries remain the same as their initial or restart values.

Specified values, $k = f$ and or $\varepsilon = f$

Values of k and ε are simply set equal to the specified values.

Specified Two-Point Gradient in Coordinate Direction, $\partial k/\partial\phi = f$ and/or $\partial\varepsilon/\partial\phi = f$

Applying $\partial k/\partial\phi = f$ at the $\xi = 0$ boundary, and using two-point one-sided differencing, gives

$$k_{1,j} = k_{2,j} - f\Delta\xi$$

At the $\xi = 1$ boundary,

$$k_{N_1,j} = k_{N_1-1,j} + f\Delta\xi$$

Analogous equations can easily be written for the η boundaries, and for $\partial\varepsilon/\partial\phi = f$.

Specified Three-Point Gradient in Coordinate Direction, $\partial k/\partial\phi = f$ and/or $\partial\varepsilon/\partial\phi = f$

Applying $\partial k/\partial\phi = f$ at the $\xi = 0$ boundary, and using three-point one-sided differencing, gives

$$k_{1,j} = \frac{(4k_{2,j} - k_{3,j} - 2f\Delta\xi)}{3}$$

At the $\xi = 1$ boundary,

$$k_{N_1,j} = \frac{(k_{N_1-1,j} - k_{N_1-2,j} + 2f\Delta\xi)}{3}$$

Analogous equations can easily be written for the η boundaries, and for $\partial\varepsilon/\partial\phi = f$.

Linear Extrapolation

Linearly extrapolating from the interior points for k at the $\xi = 0$ boundary gives

$$k_{1,j} = 2k_{2,j} - k_{3,j}$$

At the $\xi = 1$ boundary,

$$k_{N_1,j} = 2k_{N_1-1,j} - k_{N_1-2,j}$$

Analogous equations can easily be written for the η boundaries, and for linear extrapolation of ε .

Remarks

1. The "no change from initial conditions" boundary condition is applied simply by non-execution of the other boundary conditions.
2. Periodic boundary conditions are updated by setting the values of k and ε at the lower boundary equal to the corresponding values at the upper boundary.

Subroutine VORTEX		
Called by	Calls	Purpose
OUTPUT TURBBL YPLUSN		Compute magnitude of total vorticity.

Input

DXI, DETA	Computational grid spacing $\Delta\xi$ and $\Delta\eta$.
ETAX, ETAY	Metric coefficients η_x and η_y (or η_r if axisymmetric.)
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
U, V, W	Velocities u , v , and w .
XIX, XIY	Metric coefficients ξ_x and ξ_y (or ξ_r if axisymmetric.)
Y	Radial coordinate r for axisymmetric flow.

Output

VORT	Total vorticity magnitude.
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Description

Subroutine VORTEX computes the magnitude of the total vorticity vector. For two-dimensional planar flow this is defined as

$$|\vec{\Omega}| = \left| \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \right|$$

and for axisymmetric flow,

$$|\vec{\Omega}| = \left[\left(\frac{\partial w}{\partial r} + \frac{w}{r} \right)^2 + \left(\frac{\partial w}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} - \frac{\partial u}{\partial r} \right)^2 \right]^{1/2}$$

Note that, for flow without swirl, the definition for axisymmetric flow is the same as for two-dimensional planar flow.

Using the chain rule, these can be rewritten in generalized nonorthogonal coordinates. For two-dimensional planar flow,

$$|\vec{\Omega}| = |(\xi_x v_\xi + \eta_x v_\eta) - (\xi_y u_\xi + \eta_y u_\eta)|$$

and for axisymmetric flow,

$$|\vec{\Omega}| = \left[\left(\xi_r w_\xi + \eta_r w_\eta + \frac{w}{r} \right)^2 + (\xi_x w_\xi + \eta_x w_\eta)^2 + (\xi_x v_\xi + \eta_x v_\eta - \xi_r u_\xi - \eta_r u_\eta)^2 \right]^{1/2}$$

At interior points, the centered difference formula presented in Section 5.0 of Volume 1 is used to numerically compute the derivatives in the above equations. At boundary points, second-order one-sided difference formulas are used.

Subroutine YPLUSN		
Called by	Calls	Purpose
INITC KEINIT TURBCH	VORTEX	Compute the distance to the nearest solid wall.

Input

* LWALL1, LWALL2	Flags specifying wall locations for ξ and η boundaries.
MU	Effective coefficient of viscosity μ .
* N1, N2	Number of grid points N_1 and N_2 , in the ξ and η directions.
* RER	Reference Reynolds number Re_r .
RHO	Static density ρ at time level n .
VORT	Total vorticity magnitude.
X, Y	Cartesian coordinates x and y , or cylindrical coordinates x and r .

Output

DUMMY	Distance to the nearest solid wall.
YPLUSD	Nondimensional distance y^+ from the nearest solid wall.

Description

Subroutine YPLUSN computes the minimum distance to the nearest solid wall and y^+ for every grid point in the computational domain. The steps involved are as followed:

1. Call VORTEX to compute total vorticity magnitude .
2. For every grid point in the computational domain,
 3. Compute the shortest distance to each solid wall, and the corresponding wall values of the total vorticity magnitude, laminar viscosity, and density.
 4. Identify the nearest solid wall and select the corresponding minimum distance to the wall y_n , the wall total vorticity magnitude $|\Omega_{wall}|$, the wall laminar viscosity μ_{wall} , and the wall density ρ_{wall} .
 5. Compute y^+ using

$$y^+ = y_n \sqrt{\frac{Re_r |\Omega_{wall}| \rho_{wall}}{\mu_{wall}}}$$

Remarks

1. The scratch array DUMMY, from the common block DUMMY1, is used to store the minimum distance to the nearest solid wall.

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13. ABSTRACT (Maximum 200 words) A computer code called <i>Proteus 2D</i> has been developed to solve the two-dimensional planar or axisymmetric, Reynolds-averaged, unsteady compressible Navier-Stokes equations in strong conservation law form. The objective in this effort has been to develop a code for aerospace propulsion applications that is easy to use and easy to modify. Code readability, modularity, and documentation have been emphasized. The governing equations are solved in generalized nonorthogonal body-fitted coordinates, by marching in time using a fully-coupled ADI solution procedure. The boundary conditions are treated implicitly. All terms, including the diffusion terms, are linearized using second-order Taylor series expansions. Turbulence is modeled using either an algebraic or two-equation eddy viscosity model. The thin-layer or Euler equations may also be solved. The energy equation may be eliminated by the assumption of constant total enthalpy. Explicit and implicit artificial viscosity may be used. Several time step options are available for convergence acceleration. The documentation is divided into three volumes. This is the Programmer's Reference, and contains detailed information useful when modifying the program. It describes the program structure, the Fortran variables stored in common blocks, and the details of each subprogram.				
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